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OPTIMAL PULSED PUMPING FOR REMEDIATION OF AQUIFERS WHEN SORPTION IS RATE-LIMITED

DISSERTATION

Lawrence J. Schmitt
Captain, USAF

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Lawrence J. Schmitt, B.S., M.S.
Captain, USAF

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Approved:

D L Coulliette 14 Nov 97

Lt Col David L. Coulliette, Co-Chairman

Mark E. Oxley 14 Nov 97

Dr. Mark E. Oxley, Co-Chairman

Dennis W Quinn 14 NOV 97

Dr. Dennis W. Quinn

Edward Heyse 14 Nov 97

Maj Edward C. Heyse

Larry W. Burggraf 14 Nov 97

Dr. Larry W. Burggraf, Dean's Representative

Robert A. Calico Jr.

Robert A. Calico, Jr.

Dean, Graduate School of Engineering

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Lawrence Joseph Schmitt

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Abstract

A variational optimization technique is developed to acquire an optimal schedule of pulsed pumping operations for use at existing pump-and-treat aquifer remediation sites. The optimization problem is stated as a minimization of a generic management objective functional, constrained by the contaminant transport equations in two-dimensional or three-dimensional flow models which account for rate-limited sorption. The two-dimensional case is fully developed and a first-order rate equation is used to describe the transport of sorbing contaminant. The first variation provides necessary optimality conditions that must be met by any optimal solution, in turn leading to a pulsed pumping schedule of operation. The second variation provides necessary and sufficient optimality conditions that characterize the solution as minimal, maximal, or neither. General classes of functionals are examined to determine the types of objectives which can be achieved. Specific examples are presented to demonstrate how to use the method in conjunction with a numeric flow simulation, such as SUTRA.

OPTIMAL PULSED PUMPING FOR REMEDIATION OF AQUIFERS WHEN SORPTION IS RATE-LIMITED

I. Introduction

1.1 Background

Groundwater is the main source of drinking water in many regions throughout the world. Although groundwater accounts for only 0.61 percent of the earth's total water supply (22% of the land-based water), nearly 53 percent of all Americans obtain their drinking water from groundwater supplies (Fetter, 1993:1). As much as we depend on groundwater for public use, agricultural irrigation creates the largest demand on groundwater supplies -- approximately three times as much as consumed by the general population (Bedient et al., 1994:3). Obviously, groundwater is a critical natural resource.

The ecology movement of the 1970s brought to the view of the nation the great atrocities taking place on our lakes and waterways. "Lake Erie was pronounced dead, the Cyahoga River was so polluted it caught on fire, and sewage from 50 million people across the country was discharged into our waterways with little or no treatment" (Masters, 1991:101). The newly formed Environmental Protection Agency (EPA) was charged with the responsibility of maintaining and protecting the quality of our water supply, to include both surface waters and subsurface aquifers. Through legislation such

as the Clean Water Act of 1970, and the allocation of billions of dollars for wastewater treatment grants, the control of surface water pollution has been largely achieved. However, the discovery of numerous hazardous waste sites throughout the country began a new age of problems concerning the nation's water supplies. Through years of abuse, both intentional and unintentional, many subsurface aquifers are now contaminated in much the same way as the lakes and rivers of the 1970s. Many sources contribute to the contamination problem; including, among others, leaking underground storage tanks, landfills, waste-disposal injection wells, septic systems, agricultural wastes, and radioactive contaminants (Bedient et al.,1994:Ch 4). See Figure 1 for mechanisms of groundwater contamination.

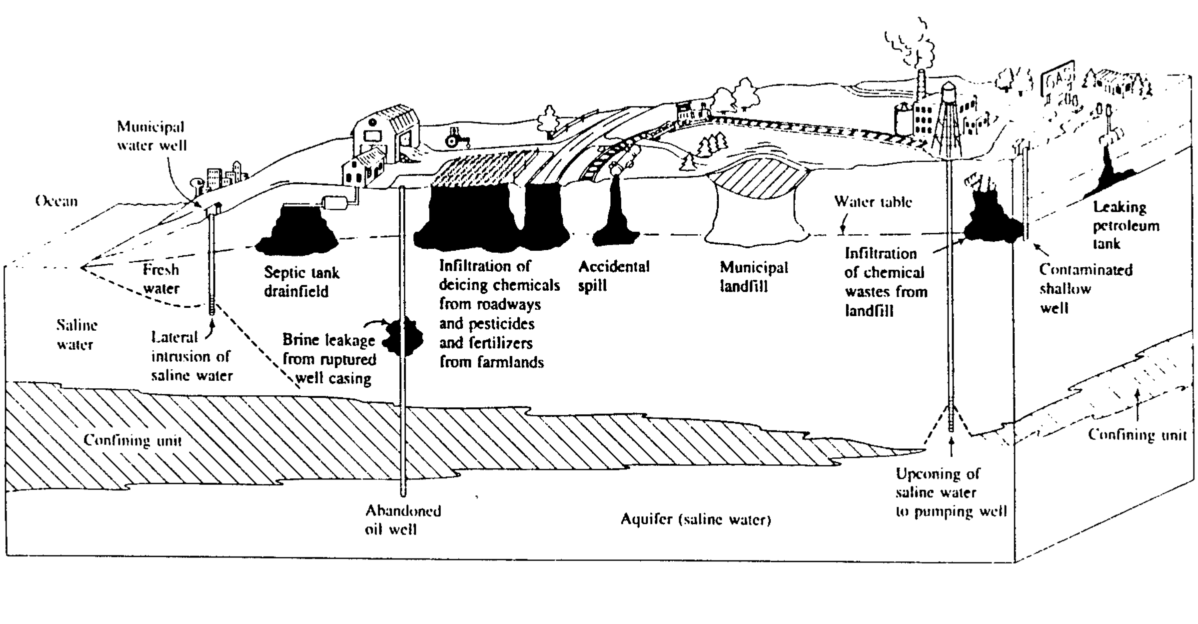

Figure 1. Mechanisms of groundwater contamination. (Source: Fetter, 1993:17).

Research by groundwater scientists and engineers has led to a number of techniques to assist in both remediation and containment of groundwater contamination. Motivated by EPA mandates such as the Resource Conservation and Recovery Act (RCRA) and the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), efficient aquifer cleanup remains an intense area of research. In general, the remediation of a site must address two major issues: source-control measures and treatment of contaminated groundwater and/or soil (Fetter, 1993:392).

Assuming that the source of the contamination has been removed, then the problem reduces to treating the groundwater/soil in order to remove or greatly reduce the contaminant concentration. Generally accepted remediation alternatives for subsurface contamination problems include:

1. Excavation and disposal of contaminated soil.
2. Containment with physical barriers.
3. Pumped removal of contaminated water and above ground treatment.
4. In situ biological or chemical treatment.
5. Soil vapor extraction.

Although the above list is not exhaustive, it represents the most prevalent and successful techniques currently being applied at hazardous-waste sites around the country (Bedient et al., 1994:421).

The third alternative listed above is commonly referred to as *pump-and-treat remediation.* Although pump-and-treat water extraction is the most commonly used remedial technology (Charbeneau et al., 1992:4), this method has failed to fully remediate

any contaminated aquifer (Travis & Doty, 1990:1465). Additionally, the concentration of contaminant in the extracted water often decreases over time and asymptotically approaches a residual level in the latter stages of remediation (Keely et al., 1987:91). This phenomena is known as *tailing*. Furthermore, in some cases concentration levels may increase after the cessation of pumping (Mackay & Cherry, 1989:633). This *rebound* effect can be attributed to the sorption of contaminants to the aquifer solids that often desorb into the aquifer years after the site has been declared safe. This sorption/desorption phenomena is referred to as rate-limited sorption. Often, sorbed contaminant mass may be on the same order or greater than the contaminant mass dissolved in the aquifer (Mackay & Cherry, 1989:632).

Volatile organic compounds (VOCs) are one of the most common health-threatening chemicals encountered at hazardous waste sites, including those which fall within the responsibility of the Air Force Installation Restoration Program (IRP). The advantage of pump-and-treat methods at sites that contain VOCs is that conventional methods of water treatment can be employed to remediate the aquifer. The treated water can then be discharged to a surface-water body, sent to a wastewater treatment plant for further treatment, or reinjected into the ground (Fetter, 1993:401). In the foreseeable future, pump-and-treat facilities will continue to operate at VOC contaminated sites. With this prediction in mind, extensive research efforts are in place to design optimal remediation strategies for effective and efficient cleanup operations. Optimization techniques are being applied to mathematical models which simulate contaminant transport at remediation sites. The results of these efforts will determine well location and

pumping rates at new cleanup sites, as well as optimal pumping schedules at existing sites.

1.2 Research Objectives

This work develops a mathematical tool incorporating contaminant transport (affected by rate-limited sorption) with a variational optimization technique to determine an optimal pulsed pumping schedule for use at an existing pump-and-treat cleanup facility. Typically, pump-and-treat groundwater remediation designs are based on trial and error simulations. Feasible combinations of pump locations and pumping rates are examined and the final design of the well-field is based on the designer's best guess. Such an approach is unlikely to be optimal (Culver & Shoemaker, 1992:629). With so many of these types of facilities already in place, the economic impact of completely redesigning these remediation projects may not be acceptable. However, the possibility of mathematically optimizing the operation of the existing facility (i.e., adjustment of pumping schedules, minor alterations in pump placement) to get the 'best bang for the buck,' could result in a significant cost reduction of Air Force and Department of Defense (DOD) remediation budgets.

For example, the impetus of this research is the IRP site at Tinker Air Force Base (AFB) Oklahoma, which is located within the recharge area of the Central Oklahoma aquifer. Since the early 1940s, industrial practices related to aircraft maintenance operations in building 3001 have resulted in contamination of surface soils and groundwater beneath and adjacent to the building. Numerous compounds including both

volatile organics and inorganic metals have been detected in the groundwater. Among these contaminants, trichloroethylene (TCE) and chromium (Cr) are the most pervasive with TCE being detected at concentrations greater than 300 ppm and Cr registering greater than 50 ppm (Battelle, 1995). Under the direction of the IRP, the Air Force constructed and began operation of a groundwater treatment facility in 1993. The pump-and-treat system consists of an extraction well-field comprised of 33 wells, five of which are horizontal, and an on-site treatment facility which treats the water to drinking water standard quality for reuse within building 3001. With the scheme currently in place, the contamination plume has been contained to a 200 acre area, approximately 200 feet below the building. Under current management plans, this operation will continue indefinitely at an operation and maintenance cost of roughly $900,000 annually. Additionally, Tinker AFB is just one of more than 1300 sites on the EPA's National Priorities List (NPL). If the current cleanup methods are going to be continued in the future, optimization of pumping schedules for cost effectiveness is critical.

The ultimate goal of this research is to develop an optimal pumping schedule for a hypothetical aquifer that will maximize the amount of contaminant removed while minimizing the cost of operating and maintaining the pumping equipment. The approach employs calculus of variations to optimize a general objective functional, constrained by the contaminant transport equations and a first-order sorption equation. With this generic approach, entire classes of functionals are examined to establish necessary and sufficient conditions for the existence of extrema.

Hartman (1994) used this methodology to establish proof of the concept in a one dimensional, radially symmetric model when contaminant transport was affected by rate-limited sorption. Hartman's work was unique in its approach to the optimization problem, in that no one had ever applied variational principles to determine if an optimal pulsed pumping schedule was attainable. However, his limiting assumptions greatly simplified the problem, creating an isolated and restricted case. In turn, these restrictions limited the scope of his conclusions. The present work examines the problem in a general geometry that provides a more realistic representation of the physical properties associated with the aquifer. Thus, this work removes the idealized geometry assumptions, and develops the theory with the mathematical rigor which Hartman's work lacked.

1.3 Relevant Terminology

Some of the significant terms used in association with contaminant transport and aquifer remediation are listed below. Unless otherwise noted, they are definitions prescribed by the EPA (U.S. EPA, 1993).

1. Advection: the process whereby solute is transported by the bulk mass of flowing fluid.

2. Aquifer: a geologic unit that contains sufficient saturated permeable material to transmit significant quantities of water.

3. Cleanup: the attainment of a specified contaminant concentration level (Goltz and Oxley, 1991:547).

4. Concentration Gradient: difference in concentration values that produces movement of a contaminant from a region of higher concentration to one of lower concentration (Freeze and Cherry, 1979:25).

5. Desorption Process: sorbed solutes reenter the aqueous phase.

6. Diffusion: mass transfer as a result of random motion of molecules.

7. Dispersion: the spreading and mixing of the contaminant in ground water due to variations in velocities within and between pores.

8. Effective Porosity: the ratio, usually expressed as a percentage, of the total volume of voids available for fluid transmission to the total volume of the porous medium.

9. Extraction Well: a pumped well used to remove contaminated groundwater.

10. Heterogeneous aquifer media: a geologic unit in which the hydrologic properties vary from point to point.

11. Homogeneous aquifer media: a geologic unit in which the hydrologic properties are identical from point to point.

12. Pulsed Pumping: a pump-and-treat enhancement where extraction wells are periodically not pumped to allow concentrations to increase in the water to be extracted.

13. Rebound: increase in contaminant concentration in the ground water that is observed due to desorption (Adams and Viramontes, 1989:1-4).

14. Retardation: the movement of a solute through a geologic medium at a velocity less than that of the flowing groundwater due to sorption or other removal of the solute.

15. Sorption: processes that remove solutes from the fluid phase and concentrate them on the solid phase of a medium.

16. Tailing: the slow, nearly asymptotic decrease in contaminant concentration in water flushed through contaminated material.

1.4 Overview

This document consists of eight chapters. Chapter II presents a review of the current literature associated with optimization of groundwater remediation. The literature review is comprised of two sections addressing two distinct areas of interest: optimal management of groundwater remediation facilities and optimal design of such facilities. The first section discusses current literature that supports the use of pulsed pumping as an optimization tool. The second section contains a review of other research efforts currently in place which use formal optimization techniques to design groundwater remediation sites.

Chapter III develops the general optimization problem and formally states the problem as a minimization of an objective functional constrained by a system of partial differential equations, initial conditions, and boundary conditions. The optimization procedure is also outlined, and the chapter includes a number of relevant definitions and theorems from the classical theory of the calculus of variations. Specifically, this chapter establishes the connection between the first and second variation with the necessary and sufficient conditions for the existence of an extremum.

Chapter IV explores the first variation of the Lagrangian of the problem presented in the preceding chapter. Basically, the Lagrangian combines the functional in question with the constraints of the problem to define a new functional. When an optimal solution

is found from the first and second variation of the Lagrangian, the solution also optimizes the original functional. In this chapter, a number of necessary conditions are derived from the first variation of the Lagrangian which reduces to a set of n-1 equations that must be satisfied to establish n-1 times to cycle (turn off or turn on) the single extraction pump. These times represent the candidate optimal solution. That is, once we verify the solution yields a minimum for a given functional, the optimal times define the best pulsed pumping schedule to attain the objectives described by the original functional.

More necessary conditions are obtained through analysis of the second variation of the Lagrangian and are presented in Chapter V. As anyone with knowledge of basic calculus and the second derivative test might expect, the necessary conditions derived from the second variation are inequality conditions which determine whether the candidate solution is a maximum, a minimum, or neither.

In Chapter VI, several definitions and theorems are presented, leading to a theorem which establishes a set of conditions, both necessary and sufficient for the existence of a minimum solution.

General classes of functionals are examined in Chapter VII, and a demonstration of the technique is also presented. By examining classes of functionals, we can determine the nature of the types of objectives that can be optimized. It turns out that some objective functionals have no optimal solution with regard to a pulsed pumping scheme. For a specific functional that has an optimal solution, a modified version of the public domain United States Geological Survey Saturated Unsaturated Transport (SUTRA) code that incorporates rate-limited sorption was used to generate concentration information at

the extraction well in a two-dimensional aquifer model (Caspers, 1994). This information was then used to determine the optimal times to switch from the pumping cycle to the resting cycle (and vice versa).

Finally, Chapter VIII summarizes the results of this research, and presents suggestions for further projects in this area.

II. Literature Review

In this chapter, the current remediation optimization literature is reviewed. Two distinct areas of interest are presented: optimal *management* of remediation facilities and optimal *design* of pump-and-treat cleanup sites. Pulsed pumping has been suggested as a possible optimization tool for existing pump-and-treat facilities, and the literature presented in the next section supports this theory. Section 2.2 examines the task of designing optimal pump-and-treat facilities with regard to pump placement and pumping rates, and the literature discusses a number of interesting possibilities.

2.1 Optimal Pump-and-treat Management Strategies

2.1.1 Introduction. Approximately two-thirds of the existing EPA Superfund groundwater contamination sites are currently being cleaned by pump-and-treat technology. Yet, not a single aquifer in the United States has ever been successfully restored by this method (Travis & Doty, 1990:1465). Cleanup objectives have not been reached, and the time needed to meet health-based requirements for groundwater quality appears to be much greater than originally anticipated. Numerous ongoing research efforts (Kuo et al., 1992; Harvey et al., 1994; Rogers & Dowla, 1994; Rogers et al., 1995) are attempting to address the problems associated with these lengthy aquifer cleanup times. Pump-and-treat methodology has been under great scrutiny, and most of the research has attempted to gain a better understanding of the method and its limitations, as well as alternative remedial strategies (Rabideau & Miller, 1994:1458).

A number of factors contribute to the lengthy cleanup times encountered by pump-and-treat systems, but the primary hindrance can be attributed to the presence of contaminant in soil regions which are not easily accessed by the flow fields generated during pumping (Rabideau & Miller, 1994:1457). Specifically, if contaminant is sorbed to the soil in the aquifer and mass transfer of contaminant between the soil and water is rate-limited, then the solute is considerably more difficult to remove.

One reason removal rates and remediation times are so poorly estimated is that most existing mathematical models assume instantaneous equilibrium between aqueous and sorbed contaminant. This local equilibrium assumption (LEA) asserts that, during pumping, sorbed contaminant instantaneously desorbs into the clean water that moves through the aquifer as contaminated water is removed. Depending upon the characteristics of both the contaminant and the soil, the LEA could be completely invalid, greatly increasing the expected time to remediate a contaminated aquifer, as predicted by the model (Goltz, 1991:25). Additionally, tailing and rebound are attributed in part to mass transfer rate limitations such as rate-limited sorption (Mackay & Cherry, 1989). Thus, the LEA could cause a significant miscalculation of groundwater cleanup times if rate-limited sorption/desorption is significant.

2.1.2 Pulsed Pumping. To address the problems associated with rate-limited sorption, Keely et al. (1987) proposed a groundwater management optimization scheme in which an intermittent or pulsed method of operation is used, in lieu of operating the extraction and injection pumps continuously. During pulsed operation, the hydraulic well system is cycled through a period of 'resting' and 'active' phases, i.e., the pumps are

turned on and off. Theoretically, resting modes of operation allow sorbed contaminant to diffuse into the more mobile regions, resulting in higher contaminant concentrations in the groundwater when the pumps are turned on (active). Since treatment costs vary directly with the amount of water pumped, the most efficient operation should remove the minimum amount of contaminated groundwater at the maximum level of contaminant concentration during the active cycle (Keely et al., 1987:99). Since operation of a remediation site could last decades, any pumping schedule that maximizes the amount of contaminant removed while minimizing the amount of water treated would result in substantial cost savings in operation budgets.

Huso (1989) developed a one-dimensional numerical model that incorporated rate-limited sorption based on a radially symmetric domain. His results verified the findings of Mackay and Cherry (1989), clearly demonstrating that cessation of pumping before a significant decrease of contaminant concentration levels in the immobile region resulted in the rebound effect previously noted. Huso recognized that pulsed pumping could address the rebound problem, but did not attempt to find an optimal pumping schedule.

Borden and Kao (1992) developed a mathematical model to simulate a groundwater extraction system for remediation of petroleum-contaminated aquifers. Continuous pump-and-treat methods are mostly ineffective when the source of contamination is a non-aqueous phase liquid (NAPL), such as petroleum (Malone et al., 1993:2203). NAPL contamination displays the same long rate of dissolution as rate-limited sorption in soils. Borden and Kao conducted simulations to evaluate the effects

of pulsed pumping in a NAPL contaminated aquifer. They developed a numerical model to compare three remediation alternatives: constant pumping rate, reduced pumping rate, and a pulsed pumping strategy. To examine the effects of pulsed pumping, they used a somewhat arbitrary schedule of pumping: pump at a constant rate for the first four years and then use a pulsed pumping schedule broken into one year increments for the next six years. They made no attempt to use mathematical optimization analysis to arrive at an optimal pumping schedule for the pump switching times. The conclusions of their research indicated that pulsed pumping resulted in a greater reduction in the contaminant concentration, however the total water volume treated appeared to be the same as in the constant pumping alternative. Borden and Kao's results demonstrated a potential for improved efficiency by using pulsed pumping, but without attempting to find an optimal pumping schedule they may have been pumping during periods when the pumps really should have been off; resulting in a less efficient pumping alternative. One disadvantage of pulsed pumping was pointed out to be the operational problems associated with restarting the pumping equipment.

Adams and Viramontes (1993) developed an analytical model of contaminant transport affected by rate-limited sorption. Their solution used a Green's function/Laplace transform approach to analytically solve the contaminant transport equations. They tested their model on a hypothetical aquifer and compared continuous pumping at a constant rate with a pulsed pumping schedule. As was the case with Borden and Kao, switching times for cycling the pump off and on were dictated arbitrarily (100 days on, 100 days off intervals for 400 days). Adams and Viramontes demonstrated that

pulsed pumping was more efficient than continuous pumping in terms of contaminant removed per treated water volume. Again, the results were rather crude, since they made no attempt to find an optimal pumping schedule.

Gorelick et al. (1993) specifically addressed the problem of optimizing the remediation of groundwater contamination sites. A number of design strategies were examined as well as techniques which could be used at existing pump-and-treat facilities. The authors recognized the attractive possibilities of using a pulsed pumping schedule rather than a continuous-on pumping approach:

> *Systematic methods for the design of pulsed-pumping networks are now becoming available. Ultimately, such methods may allow for the optimal design of pumping-rate schedules and pump/rest cycles for complex well networks, but at the present time a more operational approach must be followed (Gorelick et al., 1993:226).*

Basically, the operational approach referred to above is to monitor the water quality of the plume as remediation proceeds, then when the concentration falls and approaches a relatively low constant value, the pumps are turned off and the operator then waits for rebound to occur before restarting the pumps. However, the authors point out that even though pulsed pumping has a tremendous potential to minimize the cost of operating a pump-and-treat facility, there may be extraneous costs associated with shutting the pumps down periodically. Specifically, resting periods may induce the need for peripheral gradient measures to ensure hydrodynamic control of the plume, resulting in added costs to the remediation project.

Voudrias and Yeh (1994) investigated the factors affecting the dissolution of a toluene pool by constructing an experimental aquifer 85 cm long, 30 cm high, and 20 cm

wide. Steady-state concentration data for the aquifer was predicted by a two-dimensional advection-transverse dispersion model. They concluded pulsed pumping was more efficient than continuous pumping, as indicated by a 20% increase in mass removed per unit of water pumped and a 50% reduction in the volume of water pumped. However, their research suggested longer removal times, since a lower total mass was removed by pulsed pumping when compared with continuous pumping. The authors also pointed out that under low NAPL mass transfer limit conditions, due to the slow diffusion from the immobile regions, it may be possible to optimize the zero flow period. That is, a pulsed schedule could be developed to determine the optimal switching times resulting in higher contaminant mass removal and lower water volume extracted for treatment (Voudrias & Yeh, 1994:311). They also state that pumping and nonpumping periods can only be optimized through a trial-and-error operation, measuring the benefits with respect to plume containment.

Rabideau and Miller (1994) pointed out that very little quantitative data exists to support the conceptual theories of many alternative pump-and-treat strategies. They sought to develop efficient simulation models to accurately represent the principle flow, transport, and reaction processes influencing pump-and-treat remediation. In turn, they could then focus on evaluating the feasibility of alternative pumping strategies. They developed models incorporating LEA and rate-limited assumptions for a radially symmetric domain. After studying pulsed pumping in the rate-limited cases, they concluded that pulsed pumping increased cleanup time but this increase was offset by the improvement in remediation efficiency. After many simulations in which alternative

pumping cycles were introduced, they concluded that the best results were obtained with short pumping cycles. Additionally, they demonstrated that layered heterogeneity was very significant for pump-and-treat performance, which indicated that rebound and tailing could be observed to some extent even in the absence of rate-limited sorption.

Harvey et al. (1994) compared pulsed and continuous pumping at the design stage of a remediation facility, and clearly demonstrated that pulsed pumping was no more efficient than continuously pumping at a constant rate. However, they additionally investigated the possibility of implementing a pulsed pumping schedule at working remediation systems in order to optimize their operation, and concluded that a pulsed pumping schedule could be designed to remove the same amount of contaminant as a continuous pumping approach. By reducing overall pumping time, a savings in treatment costs could be realized at most sites.

In summary, the authors mentioned in this section recognized the potential benefit of pulsed pumping as an optimization tool, particularly when sorption was rate-limited. However, their investigations of pulsed pumping schedules used arbitrary or trial-and-error methods to explore that potential, rather than an analytical optimization technique.

2.1.3 Optimal Pulsed Pumping. While others have examined the feasibility of pulsed pumping through experiment and simulation, only Hartman (1994) attempted to use mathematical analysis to develop a pulsed pumping schedule, and he proved theoretically that an optimal schedule is obtainable on an idealized, radially symmetric geometry. Hartman depicted a hypothetical aquifer using a contaminant transport model affected by rate-limited sorption. He used variational calculus to optimize a generic

objective functional and determined necessary and sufficient optimality conditions to obtain the best pulsed pumping schedule for a specific cleanup objective. Although his research was noteworthy, in that he attempted to find an optimal schedule through a mathematical technique, he limited his efforts to a very simple component of a much more complex problem. The present research also uses a variational optimization technique, but in a much more general setting that realistically models an actual pump and treat remediation site. This generalized approach led to a more thorough and rigorous analysis of the problem, in turn establishing necessary and sufficient optimality conditions which are applicable at working remediation sites. Since Hartman's work was unique in its approach to optimal pump management, a brief summary of his work is presented here and will be referenced later in this document as a special case of the current research.

Hartman's work extended the efforts of Huso (1989), Goltz & Oxley (1991), and Adams & Viramontes (1993). Following Goltz & Oxley (1991), Hartman described contaminant transport by a steady, converging radial flow field resulting from advection created by a single extraction well. He ignored contaminant transport due to a natural groundwater gradient, and he considered the hydraulic head to be constant throughout the aquifer, thus ignoring drawdown due to pumping. Contamination was radially symmetric throughout the vertical extent of the aquifer and a full penetrating extraction well was placed in the center of the contaminated region. Hartman considered a single, infinite aquifer of constant thickness bounded below by a horizontal aquitard and assumed no other external sources or sinks of the pollutant. He modeled rate-limited

sorption/desorption between regions of mobile and immobile water by use of a first-order differential equation. Finally, he assumed the pumping schedule was piecewise constant on a fixed, finite time interval and he investigated only one pulsed pumping cycle, as shown in Figure 2.

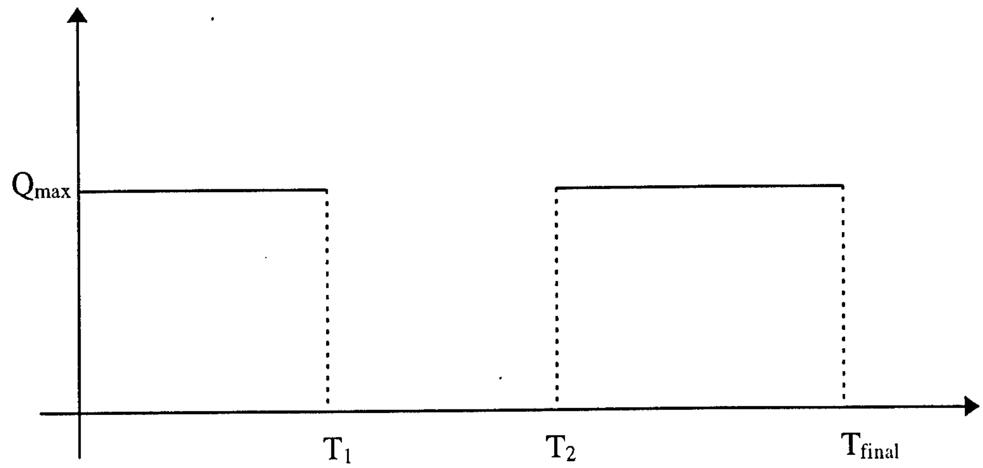

Figure 2. One cycle of a piecewise constant pumping schedule on a fixed time interval.

With these assumptions, Hartman formalized the pulsed pumping optimization problem as a minimization problem for a generic dimensionless objective functional, $J[Q,C_m]$, subject to the constraints posed by the contaminant transport equations and the geometry of the aquifer domain as follows:

- Minimize $$J[Q,C_m] = \int_0^{T_{final}} f(T,Q(T),C_m(X_w,T))dT \qquad (1)$$

over the piecewise constant set of functions $S = \{Q: [0,T_{final}] \rightarrow \{0,Q_{max}\}$ and Q is piecewise constant$\}$, where C_m, Q, X_w, and T are dimensionless variables that represent concentration in the mobile zone, extraction well pumping rate, coordinate location of the

well, and time, respectively. The integrand f given in equation (1) was intentionally left generic to let an aquifer manager choose the desired objective functional (i.e., f might be chosen to maximize contaminant mass removed while minimizing the mass of water removed, or some other management goal) defined over a finite time interval, $[0, T_{final}]$.

- Subject to the constraints

$$\frac{\partial C_m(X,T)}{\partial T} = \left(\frac{Q(T)}{X} + D\right)\frac{\partial^2 C_m(X,T)}{\partial X^2} + \left(\frac{Q(T)}{X} + \frac{D}{X}\right)\frac{\partial C_m(X,T)}{\partial X} - \beta\frac{\partial C_{im}(X,T)}{\partial X} \quad (2)$$

and

$$\frac{\partial C_{im}(X,T)}{\partial T} = \alpha\left[C_m(X,T) - C_{im}(X,T)\right] \quad (3)$$

where C_{im} represents the dimensionless concentration in the immobile zone, and D, α, and β are dimensionless constants. The initial conditions were specified as

$$C_m(X,0) = C_{m,o}(X) = \begin{cases} 1 & \text{for} \quad X_w < X < X_* \\ 0 & \text{for} \quad X_* < X < \infty \end{cases} \quad (4)$$

and

$$C_{im}(X,0) = C_{im,o}(X) = \begin{cases} 1 & \text{for} \quad X_w < X < X_* \\ 0 & \text{for} \quad X_* < X < \infty \end{cases}, \quad (5)$$

where X_* was some finite radius which defined the contaminated region. Also, the boundary conditions were defined as

$$\frac{\partial C_m}{\partial X}(\infty,T)+C_m(\infty,T)=0 \quad \text{and} \quad C_m(\infty,T)=0 \quad \text{for all} \quad T\in[0,T_{final}] \tag{6}$$

$$\frac{\partial C_{im}}{\partial X}(\infty,T)+C_m(\infty,T)=0 \quad \text{and} \quad C_{im}(\infty,T)=0 \quad \text{for all} \quad T\in[0,T_{final}]. \tag{7}$$

At this point, Hartman applied the classical calculus of variations approach (see, for example, Gelfand & Fomin (1963)), and arrived at necessary and sufficient optimality conditions for the first and second variations of the functional in (1). His work is summarized by the following theorems:

Theorem (Necessary Optimality Conditions for the First Variation). Let $J[Q, C_m]$ be the functional given by equation (1), constrained by the partial differential equations, boundary conditions, and initial conditions given in (2) through (7), and assume that f has continuous first and second partial derivatives for all its variables on $[0, T_{final}]$. Define

$$Q(T)=\begin{cases}1 & 0<T<T_1\\ 0 & T_1<T<T_2\\ 1 & T_2<T<T_{final}\end{cases},$$

and

$$C_m(X_w,T)=\begin{cases}C_m^{(1)}(X_w,T) & 0<T<T_1\\ C_m^{(2)}(X_w,T) & T_1<T<T_2\\ C_m^{(3)}(X_w,T) & T_2<T<T_{final}\end{cases}.$$

If the functions $(\hat{Q},\hat{C}_m)$ produce an extremal for the functional in (1) constrained by (2) through (7), then

$$\begin{aligned} & f\left[\hat{T}_1,1,\hat{C}_m^{(1)}(X_w,\hat{T}_1)\right]-f\left[\hat{T}_1,0,\hat{C}_m^{(2)}(X_w,\hat{T}_1)\right] \\ & \quad -\hat{C}_m^{(1)}(X_w,\hat{T}_1)\frac{\partial f}{\partial C}\left[\hat{T}_1,1,\hat{C}_m^{(1)}(X_w,\hat{T}_1)\right]+\hat{C}_m^{(2)}(X_w,\hat{T}_1)\frac{\partial f}{\partial C}\left[\hat{T}_1,0,\hat{C}_m^{(2)}(X_w,\hat{T}_1)\right]=0 \end{aligned} \tag{8}$$

and

$$
\begin{aligned}
&f[\hat{T}_2, 0, \hat{C}_m^{(2)}(X_w, \hat{T}_2)] - f[\hat{T}_2, 1, \hat{C}_m^{(3)}(X_w, \hat{T}_2)] \\
&\quad - \hat{C}_m^{(2)}(X_w, \hat{T}_2)\frac{\partial f}{\partial C}[\hat{T}_2, 0, \hat{C}_m^{(2)}(X_w, \hat{T}_2)] + \hat{C}_m^{(3)}(X_w, \hat{T}_2)\frac{\partial f}{\partial C}[\hat{T}_2, 1, \hat{C}_m^{(3)}(X_w, \hat{T}_2)] = 0
\end{aligned}
\tag{9}
$$

must hold, where $\hat{T}_1$ and $\hat{T}_2$ represent the optimal pump switching times produced by the functions $(\hat{Q}, \hat{C}_m)$.

With the initial assumption of only one cycle of pulsed pumping, $\hat{T}_1$ was the optimal time to turn the pump off and $\hat{T}_2$ was the optimal time to turn the pump back on. Additionally, Q(T) = 1 means the pump is on and Q(T) = 0 means the pump is off. Finally, note that $\hat{C}_m^{(1)}(X_w, \hat{T}_1)$ denotes the concentration observed at the well at the instant the pump is turned off, and $\hat{C}_m^{(2)}(X_w, \hat{T}_2)$ denotes the concentration observed at the well at the instant the pump is turned back on.

Theorem (Necessary Optimality Conditions for the Second Variation). Define $J[Q, C_m]$, $Q(T)$, and $C_m(X_w, T)$ as in the previous theorem. If the functions $(\hat{Q}, \hat{C}_m)$ produce an extremal for the functional in (1) constrained by (2) through (7), then

$$
\frac{\partial^2 f}{\partial C^2}[T, \hat{Q}(T), \hat{C}_m(X_w, T)] \geq 0 \tag{10}
$$

for all $T \in [0, T_{final}]$, and

$$
\begin{aligned}
&\frac{\partial f}{\partial T}[\hat{T}_1, 1, \hat{C}_m^{(1)}(X_w, \hat{T}_1)] - \frac{\partial f}{\partial T}[\hat{T}_1, 0, \hat{C}_m^{(2)}(X_w, \hat{T}_1)] \\
&+ \hat{C}_m^{(1)}(X_w, \hat{T}_1)\left\{ -\frac{\partial^2 f}{\partial T \partial C}[\hat{T}_1, 1, \hat{C}_m^{(1)}(X_w, \hat{T}_1)] - \frac{\partial^2 f}{\partial C^2}[\hat{T}_1, 1, \hat{C}_m^{(1)}(X_w, \hat{T}_1)]\frac{\partial \hat{C}_m^{(1)}}{\partial T}(X_w, \hat{T}_1) \right\} \\
&- \hat{C}_m^{(2)}(X_w, \hat{T}_1)\left\{ -\frac{\partial^2 f}{\partial T \partial C}[\hat{T}_1, 0, \hat{C}_m^{(2)}(X_w, \hat{T}_1)] - \frac{\partial^2 f}{\partial C^2}[\hat{T}_1, 0, \hat{C}_m^{(2)}(X_w, \hat{T}_1)]\frac{\partial \hat{C}_m^{(2)}}{\partial T}(X_w, \hat{T}_1) \right\} \geq 0
\end{aligned}
$$

(11)

and

$$\frac{\partial f}{\partial T}[\hat{T}_2,0,\hat{C}_m^{(2)}(X_w,\hat{T}_2)]-\frac{\partial f}{\partial T}[\hat{T}_2,1,\hat{C}_m^{(3)}(X_w,\hat{T}_2)]$$
$$+\hat{C}_m^{(2)}(X_w,\hat{T}_2)\left\{-\frac{\partial^2 f}{\partial T\partial C}[\hat{T}_2,0,\hat{C}_m^{(2)}(X_w,\hat{T}_2)]-\frac{\partial^2 f}{\partial C^2}[\hat{T}_2,0,\hat{C}_m^{(2)}(X_w,\hat{T}_2)]\frac{\partial \hat{C}_m^{(2)}}{\partial T}(X_w,\hat{T}_2)\right\}$$
$$-\hat{C}_m^{(3)}(X_w,\hat{T}_2)\left\{-\frac{\partial^2 f}{\partial T\partial C}[\hat{T}_2,1,\hat{C}_m^{(3)}(X_w,\hat{T}_2)]-\frac{\partial^2 f}{\partial C^2}[\hat{T}_2,1,\hat{C}_m^{(3)}(X_w,\hat{T}_2)]\frac{\partial \hat{C}_m^{(3)}}{\partial T}(X_w,\hat{T}_2)\right\}\geq 0$$
(12)

must hold, where $\hat{T}_1$ and $\hat{T}_2$ represent the optimal pump switching times produced by the functions $(\hat{Q},\hat{C}_m)$.

Theorem (Sufficient Optimality Conditions for the Second Variation). If the functions $(\hat{Q},\hat{C}_m)$ are an extremal for the functional given by equation (1), constrained by the partial differential equations, boundary conditions, and initial conditions given in (2) through (7) (that is, equations (8) and (9) are satisfied), and

$$\frac{\partial^2 f}{\partial C^2}[T,\hat{Q}(T),\hat{C}_m(X_w,T)]>0 \tag{13}$$

for all $T\in[0,T_{\text{final}}]$,

$$\frac{\partial f}{\partial T}[\hat{T}_1,1,\hat{C}_m^{(1)}(X_w,\hat{T}_1)]-\frac{\partial f}{\partial T}[\hat{T}_1,0,\hat{C}_m^{(2)}(X_w,\hat{T}_1)]$$
$$+\hat{C}_m^{(1)}(X_w,\hat{T}_1)\left\{-\frac{\partial^2 f}{\partial T\partial C}[\hat{T}_1,1,\hat{C}_m^{(1)}(X_w,\hat{T}_1)]-\frac{\partial^2 f}{\partial C^2}[\hat{T}_1,1,\hat{C}_m^{(1)}(X_w,\hat{T}_1)]\frac{\partial \hat{C}_m^{(1)}}{\partial T}(X_w,\hat{T}_1)\right\}$$
$$-\hat{C}_m^{(2)}(X_w,\hat{T}_1)\left\{-\frac{\partial^2 f}{\partial T\partial C}[\hat{T}_1,0,\hat{C}_m^{(2)}(X_w,\hat{T}_1)]-\frac{\partial^2 f}{\partial C^2}[\hat{T}_1,0,\hat{C}_m^{(2)}(X_w,\hat{T}_1)]\frac{\partial \hat{C}_m^{(2)}}{\partial T}(X_w,\hat{T}_1)\right\}>0$$
(14)

and

$$\frac{\partial f}{\partial T}[\hat{T}_2,0,\hat{C}_m^{(2)}(X_w,\hat{T}_2)]-\frac{\partial f}{\partial T}[\hat{T}_2,1,\hat{C}_m^{(3)}(X_w,\hat{T}_2)]$$
$$+\hat{C}_m^{(2)}(X_w,\hat{T}_2)\left\{-\frac{\partial^2 f}{\partial T\partial C}[\hat{T}_2,0,\hat{C}_m^{(2)}(X_w,\hat{T}_2)]-\frac{\partial^2 f}{\partial C^2}[\hat{T}_2,0,\hat{C}_m^{(2)}(X_w,\hat{T}_2)]\frac{\partial\hat{C}_m^{(2)}}{\partial T}(X_w,\hat{T}_2)\right\}$$
$$-\hat{C}_m^{(3)}(X_w,\hat{T}_2)\left\{-\frac{\partial^2 f}{\partial T\partial C}[\hat{T}_2,1,\hat{C}_m^{(3)}(X_w,\hat{T}_2)]-\frac{\partial^2 f}{\partial C^2}[\hat{T}_2,1,\hat{C}_m^{(3)}(X_w,\hat{T}_2)]\frac{\partial\hat{C}_m^{(3)}}{\partial T}(X_w,\hat{T}_2)\right\}>0 \tag{15}$$

then the functional in (1), constrained by (2) through (7), has a minimum at $(\hat{Q},\hat{C}_m)$.

Equations (8) through (15) provided the tools to develop an optimal pulsed pumping schedule, under the assumptions listed. Once a quantity to be minimized had been selected, the specific objective could be modeled by the functional of equation (1) and these equations were then applied to derive the desired pumping schedule. With discrete values of the concentrations found from some model, equations (8) and (9) could be used to find candidate times $\hat{T}_1$ and $\hat{T}_2$ which provided an optimal solution. Equations (10) through (15) could then be applied to verify the solution was indeed a minimum.

Despite Hartman's simplifying assumptions that idealized the problem and the fact that he never actually applied his results to a nontrivial example, his work demonstrated the potential for this approach in a more general setting. The present work provides the analysis of the more general problem and demonstrates that Hartman's work serves as a special case of the general problem.

2.1.4 Summary. In this section of the literature review, an alternative groundwater management strategy known as pulsed pumping was examined. Although a number of researchers have examined the concept of pulsed pumping, very little mathematical analysis has been presented to substantiate the claim that intermittent

pumping could be used to optimize the remediation of contamination sites. While others have used "best-guess" optimization techniques to determine optimal on/off pump cycling times, only Hartman (1994) has actually sought to use a mathematical technique to truly find a best pumping schedule.

Whereas very little mathematical analysis has been applied to the pulsed pumping/scheduling concept, extensive research has been conducted to examine the feasibility of designing optimal pump-and-treat systems (assuming pump placement as a variable). A detailed examination of some of these ideas follows in the next section.

2.2 *Optimal Pump-and-treat Design Strategies*

2.2.1 Introduction. Optimization techniques have been applied to groundwater management to address both quantity of groundwater availability and quality of the groundwater purity. In his review of groundwater management modeling methods, Gorelick (1983) pointed out that although a number of methods had been used to optimize groundwater quantity, the task of applying optimization to groundwater quality models was much more formidable. The mathematical and computational complexity of the large systems of nonlinear equations generally associated with flow and contaminant transport models contributes to the difficulty of the optimization problem. Unfortunately, the simplifying assumptions needed to eliminate these nonlinearites usually limits the accuracy and usefulness of the transport model (Culver & Shoemaker, 1992:629).

In the early days of groundwater remediation, the most effective techniques in use were designed to contain a contaminant plume and prevent its migration into regional

groundwater supplies until remediation strategies could be developed. In the past ten years, a great deal of the research effort aimed at optimizing the pump-and-treat remediation method has been geared toward designing optimal cleanup facilities, addressing well placement and pumping rate selection techniques that will ultimately extract the contaminant plume. Although the research presented in this document focused on optimal pump scheduling, for completeness this section of the literature review will examine some of the techniques currently being explored to design efficient systems for management of groundwater quality.

2.2.2 Optimal Design of Pump-and-treat Sites. Initially, mathematical optimization was used to minimize pumping during containment of the contamination plume. These early plume management strategies included constraints on heads, gradients, and flow velocities, but they failed to account for concentration or cleanup time (Greenwald & Gorelick, 1989:74). Eventually, researchers recognized the need to find efficient ways to actually remediate contaminated aquifers.

Lefkoff and Gorelick (1985) designed a groundwater model that linked flow simulation and mathematical optimization. The purpose of their research was to determine if an optimal design criteria could be established to meet a target cleanup date. They examined a hypothetical aquifer which fixed the locations of the extraction and injection wells, and examined the effects of varying the pumping rates of each. Their remediation goal was to completely restore a contaminated aquifer in a four year period, and they determined the cost impact associated with such a time constraint. The desired objective was to minimize variable pumping costs, and the model they developed used a

response matrix technique. The model identified sets of decisions on pumping and injection rates, thus satisfying velocity constraints at the plume perimeter, as well as head constraints at pumping and injection sites. Their results clearly demonstrated the expense of rapid restoration, but their study also served to demonstrate the usefulness of a groundwater simulation-optimization model. In their work, Lefkoff and Gorelick examined the effects of varying a continuous pumping schedule and did not address the possibility of an optimal schedule through pulsed pumping.

Ahlfeld et al. (1988) conducted a two-part study that explored groundwater remediation through the use of simulation, optimization, and sensitivity theory. In the first part, they proposed two nonlinear optimization formulations which modeled the design of an aquifer cleanup system to decide the location and pump rates for an extraction/injection well-field. Their model combined optimization with a two-dimensional Galerkin finite element model to simulate steady state groundwater flow and transient convective-dispersive transport. The discrete concentration levels from this model served as the input to the optimization problem. The formulations were designed to find the optimal pumping configuration to either remove the most contaminant over a fixed time interval or to reach a specified contaminant level at the least cost. The discrete objective functions they used were constrained by a variety of physical and economic limitations, where the end product could either: (1) select a pumping strategy to minimize the total amount of contaminant in an aquifer after a set time period, or (2) meet some prescribed EPA standard with a minimum cost. With these tools in place, the next part of their study dealt with a real-life application of their findings. Ahlfeld et al. (1988)

demonstrated the validity of the model by investigating a series of hypothetical remediation design problems applied to a simplified field scale model of the Superfund site at Woburn, Massachusetts. Through the use of their optimization algorithm, they determined remediation strategies which satisfied specific design criteria. Additionally, their methods were found to produce engineering design information not available by any other method of analysis.

Greenwald and Gorelick (1989) investigated the adverse effects associated with implementing a rapid aquifer restoration project. Their contaminant transport model was extremely simplified; basing transport travel time purely on advective flow. They utilized an existing quasi-analytical solution for this model in combination with nonlinear optimization to determine pumping and injection rates. The discrete objective function they minimized could represent any function of pumping rates, injection rates, and cleanup time. Applying their technique, they demonstrated the importance of cleanup time as a management consideration at the design stage of an aquifer restoration system. Also, they concluded that increased pumping rates could result in increased cleanup times, thereby driving remediation costs higher. Unfortunately, the simplicity of the flow model greatly limited its usefulness.

Ahlfeld & Sawyer (1990) developed simulation and optimization techniques to determine optimal well locations. Their work was similar to that done by Lefkoff & Gorelick (1985), except that in their approach, Ahlfeld and Sawyer (1990) allowed for explicit control of groundwater velocity direction and magnitude, whereas Lefkoff and Gorelick proposed that the flow system was constrained by requirements on the

groundwater velocity. This difference allowed the user the flexibility of specifying the exact direction of the velocity vector in a particular finite element. Optimization was accomplished through the use of a two-dimensional simulation model of groundwater flow and contaminant transport. The solution of this model was generated using linear quadrilateral finite elements, and the solution data was then used to generate the response matrix. In turn, the equations produced by this matrix served as constraints to a linear program algorithm. The major advantage of this technique was that the response matrix was structured, reducing computational and storage requirements significantly. Using this approach on a hypothetical aquifer, Ahlfeld and Sawyer demonstrated that providing a greater choice of well locations produced as much as a 37% reduction in pumping costs, illustrating the importance of careful selection of well position in an aquifer cleanup site.

Dougherty and Marryott (1991 & 1993) and Kuo et al. (1992) independently investigated groundwater remediation design problems by applying the method of simulated annealing. Simulated annealing is a random-search technique that offers some advantages over continuous optimization techniques. These advantages include the ability to handle nonsmooth objective functions and the computational savings of not requiring functional gradients. However, the methods chief disadvantage is that only a limited number of pumping rates can be considered in the optimization (Xiang et al., 1995:172). In both of their approaches, potential well locations discretely defined and extraction pumping rates continuously defined were both treated as discrete combinatorial variables. Dougherty and Marryott (1991 & 1993) sought to develop two different optimization formulations; the first sought to reduce contaminant concentrations while

the second sought to contain a contaminant plume. The first formulation produced a solution that reduced pumping costs, while the second was computationally more effective. Kuo et al. (1992) had similar optimization formulations, and of particular interest, they chose 'bang-bang'- like controls (i.e. pump on, pump off) to determine optimal pump-and-treat strategies for groundwater remediation. Both groups demonstrated success with the simulated annealing model, but there focus was on pump placement. They also acknowledged the limitations due to the stochastic nature of simulated annealing.

Rogers, Dowla, and Johnson have recently generated a series of papers (Rogers & Dowla, 1994; Rogers, et al., 1995; and Johnson & Rogers, 1995) that explored a new approach to nonlinear groundwater management methodology. They sought to optimize aquifer remediation with the aid of artificial neural networks (ANNs). With the use of ANN technology, they found that solute transport simulations could be run in parallel thus achieving super-computer speed on conventional work stations. Optimal groundwater management solutions were found by training an ANN to predict the outcome of a two-dimensional hybrid finite-difference/finite-element flow and transport code, and then they used the trained network to search through many possible pumping alternatives to find an optimal realization for successful remediation. Back propagation was used to train the network, and the conjugate gradient method was used to speed convergence. A simple genetic algorithm directed the search, and the results were consistent with those found from the more conventional optimization technique of nonlinear programming with a quasi-Newton search (Rogers & Dowla, 1994:457).

Johnson and Rogers (1995) applied the neural network technique to optimal pump location analysis at a western Superfund site. After extensive characterization and analysis of the site, a 28-location pump-and-treat extraction/injection system was believed to be capable of containing and remediating the contamination within 50 years. The proposed management objective was to obtain the lowest cost subset of these 28 locations which could contain the contamination and extract the same mass of contaminant as the full 28-location strategy in the 50 year period. ANNs were trained by the 2-D SUTRA model to predict mass extraction and contamination information. Then, the networks examined over 4 million possible pump location patterns to identify 250 which met restoration goals at minimum cost. Sensitivity analysis was then used to sift through these 250 alternatives and evaluate the optimization results. The primary gain achieved through the use of ANNs was the speed at which alternative strategies could be examined; almost a million times faster than using the original SUTRA model to examine all 4 million patterns.

Ahlfeld et al. (1995) applied a hydraulic control optimization model to a groundwater remediation system at a Superfund site in coastal New Jersey. They proposed an application of a simulation/optimization approach to an actual field site that uses optimization throughout the design process. With this approach, the system designer could assess the feasibility of certain management concepts and prepare the final design based on close interaction with the decision makers. Specifically, the management problem they addressed was to devise a remediation strategy that will capture a large volume of contaminant mass while allowing recharge of all extracted and treated water to

the subsurface. The data obtained from the optimization formulation was used to determine the feasibility of the recharge concept given the complex hydraulic constraints associated with the site. Additionally, the formulation was used to analyze the pumping strategy to determine the most practical way to implement the design under realistic conditions. This study demonstrated the importance of incorporating optimization at every stage of the design phase.

2.2.3 Summary. A great deal of research has been conducted that addresses the problem of optimizing groundwater quality. This section of the literature review examined a few of the techniques currently being used to design optimal pump-and-treat remediation systems. Typically, the models used to simulate contaminant transport have been a simplified advection model or advection-dispersion equations with no accounting for the possible effects of rate-limited sorption or layered heterogeneity. Additionally, mathematical optimization methods have mostly been applied at the design stage; searching for optimal pump placement and flow rates.

2.3 Conclusion

This chapter presented the current literature dealing with optimization techniques applied to *managing* pump-and-treat groundwater cleanup facilities as well as those techniques used to optimally *design* such facilities. Specifically, pulsed pumping was presented as an alternative to continuous pumping at existing locations as a method for optimizing the operation of a site. Additionally, the literature clearly indicated that

during the design stage of a pump-and-treat cleanup facility, pulsed pumping is no more efficient than continuously pumping at a constant rate.

The research presented in this document will present an optimization procedure which, when applied at an existing pump-and-treat site, can be used to design an optimal pumping schedule for the pumps already in place. The procedure applies variational calculus to a functional on either a two- or three-dimensional domain (independent of the choice of coordinate system), constrained by the physical properties which limit contaminant transport and non-equilibrium sorption.

The next chapter of this document highlights the variational methodology which led to an optimal pulsed pumping solution. The chapter includes a statement of the optimization problem as well as the pertinent theory behind the classical calculus of variations approach, including definitions and theorems that guarantee an optimal solution.

III. Variational Methodology

3.1 Introduction and Overview

Costs to remediate contaminated aquifers have continued to escalate, and an effective cleanup methodology remains nonexistent. The prevalent technology of pump-and-treat provides for the containment of contaminant but this method could take 50 years or longer to completely restore a site to an environmentally sound condition. With the prospect of spending billions of dollars on restoration, researchers have investigated the possibility of improving the efficiency of pump-and-treat system design and operation. One such cost-cutting measure that has been proposed calls for intermittent pumping that allows desorption of contaminant from less mobile regions into more mobile regions during idle pump periods, resulting in reduced operating costs. The work presented in this document developed a mathematical tool which incorporated contaminant transport within a variational optimization technique to obtain an optimal pulsed pumping schedule at an existing pump-and-treat cleanup site. Specifically, application of variational calculus established necessary and sufficient conditions for the existence of an optimal pumping schedule.

The preceding chapters indicated support for pulsed pumping as a means to optimize operating efficiency of many restoration sites. Hartman's work (1994) proved that optimization could be achieved in an idealized, radially symmetric aquifer by use of a calculus of variations technique. In the present work, the variational technique was used

to prove that necessary and sufficient optimality conditions existed on two- and three-dimensional aquifer domains, with more realistic assumptions.

The remainder of this chapter presents an overview of the analysis developed in the following chapters. The next section lists the assumptions made in the transport model and presents the governing equations for advective-dispersive transport, coupled with a first-order sorption model. These equations serve as constraints to the optimization problem, as stated in section 3.3. Section 3.4 states the pertinent theorems and definitions needed in the analysis that follows. Finally, section 3.5 summarizes a plan of attack for this research that pursues the theory presented in 3.4.

3.2 Governing Equations

The following physical assumptions were used to develop the transport model:

1. A single extraction well was assumed to create a steady state flow field. Additionally, this single extraction well served as the contaminant concentration observation point during the analysis. Assuming a single extraction well simplified the analysis and if we assume the pumps in a well field operate independently, the procedure could easily be extended to a multiple pump system.
2. The confined aquifer and the contaminated region were assumed to have a general rectangular geometry in two and three dimensions (i.e. not radially symmetric), and the media was assumed heterogeneous and isotropic. Also, initial and boundary conditions reflected this general geometry.

3. No external contaminant sources or sinks were present, thus a finite initial concentration level was assumed.
4. A piecewise constant, pulsed pumping schedule was assumed on a fixed, finite time interval, $[0, t_f]$, that allowed for 'n' on/off intervals of varying length (see Figure 3.).
5. Rate-limited sorption/desorption was modeled within the aquifer with a first-order rate equation (van Genuchten and Wierenga, 1976; Goltz and Oxley, 1991). As observed in the literature review, many researchers link pulsed pumping strategy with rate-limited sorption, although similar benefits may result in extremely heterogeneous aquifers (Rabideau and Miller, 1994:1457).

These flow and transport assumptions are typical for many remediation problems. Later analysis showed, however, that many of these assumptions could be relaxed within the variational approach. Since the necessary and sufficient optimality conditions only required knowledge of the concentration at the observation well, any general transport model that incorporates first-order rate-limited sorption would be suitable.

The equations for advective-dispersive contaminant transport, coupled with the first-order rate expression are written as

$$\frac{\partial c}{\partial t} = \nabla \cdot (\underline{\underline{D}}_h \cdot \nabla c) - \nabla \cdot (vc) - \frac{\rho_B}{\theta} \frac{\partial s}{\partial t} \tag{16}$$

and

$$\frac{\partial s}{\partial t} = \alpha(K_d c - s), \tag{17}$$

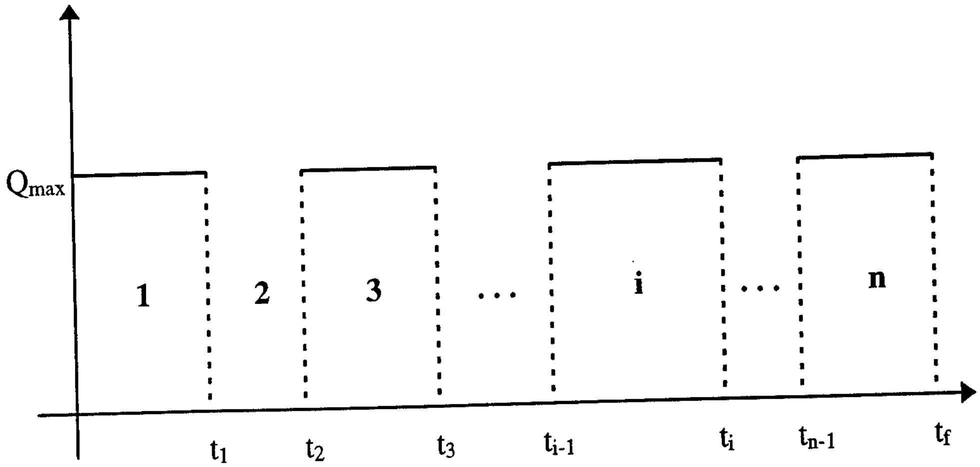

Figure 3. Piecewise constant pulsed pumping schedule on a fixed, finite time interval with n intervals of variable length.

where c(**x**,t) is the contaminant concentration of the water phase [M/L^3], s(**x**,t) is the sorbed contaminant concentration [dimensionless], **x** is a rectangular coordinate point [L], t is time [T], ρ_B is the bulk density [M/L^3], θ is the porosity of the water phase [dimensionless], α is a first-order rate constant [T^{-1}], K_d is a distribution coefficient [L^3/M], $\underline{\underline{D}}_h$ is the hydrodynamic dispersion tensor [L^2/T], given for isotropic media in two dimensions as

$$\underline{\underline{D}}_h = \begin{bmatrix} \alpha_L|\mathbf{v}| + D^* & 0 \\ 0 & \alpha_T|\mathbf{v}| + D^* \end{bmatrix} \tag{18a}$$

and in three dimensions as

$$\underline{\underline{D}}_h = \begin{bmatrix} \alpha_L|\mathbf{v}| + D^* & 0 & 0 \\ 0 & \alpha_T|\mathbf{v}| + D^* & 0 \\ 0 & 0 & \alpha_T|\mathbf{v}| + D^* \end{bmatrix}, \tag{18b}$$

where α_L and α_T are the longitudinal and transverse dispersivities of the porous medium, respectively [L], D^* is the molecular diffusion coefficient [L^2/T], and $|\mathbf{v}|$ is the magnitude of the fluid velocity vector $\mathbf{v}$ [L/T], determined by the head equation given as

$$\mathbf{v} = -\frac{1}{\theta}\underline{\underline{K}}\nabla h, \tag{19}$$

where $\underline{\underline{K}}$ is the hydraulic conductivity tensor of the medium [L/T] and h is the hydraulic head [L].

The advection-dispersion model (16) presented by Bear and Verruijt (1987:Ch 6) will be used throughout this document. For the purpose of this research, a very general transport model would be sufficient, but the model depicted by (16) and (17) was chosen because it was common in the literature and it made the analysis easier to follow. Additionally, the model equations also account for the effects of rate-limited desorption of contaminant between the sorbed and aqueous phases. The coupled equations, (16) and (17), describe the transport process and provide the partial differential equations for the boundary-value problem (BVP) which constrains the objective functional of the optimization problem (section 3.3). The boundary conditions for the BVP are

$$(\underline{\underline{D}}_h \cdot \nabla c)\cdot \hat{\mathbf{n}} = 0 \qquad \text{on} \quad B_w \tag{20a}$$

and

$$(\mathbf{v}c - \underline{\underline{D}}_h \cdot \nabla c)\cdot \hat{\mathbf{n}} = 0 \qquad \text{on} \quad B_d, \tag{20b}$$

where B_w is the *boundary* of the extraction well and B_d is the boundary of the aquifer domain. Notice, the dimension for the geometry of the domain is left arbitrary to this point. The boundary condition in (20a) implies that the concentration at the well does not change due to hydrodynamic dispersion and (20b) is the zero flux condition at the boundary of the aquifer. Finally, the initial conditions are expressed as

$$c(\mathbf{x},0) = c_0(\mathbf{x}) \tag{21a}$$

and

$$s(\mathbf{x},0) = s_0(\mathbf{x}), \tag{21b}$$

where c_0 and s_0 are the initial contaminant concentrations in the aqueous and solid phases at any point $\mathbf{x}$ throughout the domain of the aquifer, denoted in general as D.

In the statement of the optimization problem, the transport equations stated in (16) and (17) will be treated as finite subsidiary conditions (constraints) imposed on the admissible functions for which the stated objective functional has an extremum. As such, the constraints are less cumbersome when combined into a single equation. Thus, introducing the integrating factor $e^{\alpha t}$ into equation (17), an expression for the sorbed concentration is found as

$$s(\mathbf{x},t) = e^{-\alpha t} s_0(\mathbf{x}) + \alpha K_d e^{-\alpha t} \int_0^t c(\mathbf{x},\tau) e^{\alpha\tau} d\tau. \tag{22}$$

Combining equations (16), (17), and (22) and denoting the partial derivative of the concentration with respect to time as a subscript t $\left(c_t = \dfrac{\partial c}{\partial t} \right)$, then we have

$$\nabla \cdot (\underline{\underline{D}}_h \cdot \nabla c) - \nabla \cdot (\mathbf{v}c) - \frac{\rho_B \alpha K_d}{\theta} c + \frac{\rho_B \alpha}{\theta} e^{-\alpha t} s_0(\mathbf{x}) + \frac{\rho_B \alpha^2 K_d}{\theta} e^{-\alpha t} \int_0^t c(\mathbf{x},\tau) e^{\alpha\tau} d\tau - c_t = 0. \tag{23}$$

3.3 *Optimization Problem Statement*

With the derivation of equation (23), the optimization problem can now be stated:

Minimize
$$J[Q,c] = \int_0^{t_f} \int_{B_w} f(t, Q(t), c(\mathbf{x},t), c_t(\mathbf{x},t)) dB_w dt \tag{24}$$

constrained by the boundary value problem, satisfying the integro-differential equation

$$\nabla \cdot (\underline{\underline{D}}_h \cdot \nabla c) - \nabla \cdot (\mathbf{v}c) - \frac{\rho_B \alpha K_d}{\theta} c + \frac{\rho_B \alpha}{\theta} e^{-\alpha t} s_0(\mathbf{x}) + \frac{\rho_B \alpha^2 K_d}{\theta} e^{-\alpha t} \int_0^t c(\mathbf{x},\tau) e^{\alpha\tau} d\tau - c_t = 0 \tag{25}$$

in D x [0, t_f], with the boundary conditions given as

$$(\underline{\underline{D}}_h \cdot \nabla c) \cdot \hat{\mathbf{n}} = 0 \qquad \text{on } B_w \tag{26a}$$

$$(\mathbf{v}c - \underline{\underline{D}}_h \cdot \nabla c) \cdot \hat{\mathbf{n}} = 0 \qquad \text{on } B_d, \tag{26b}$$

and the initial conditions given as

$$c(\mathbf{x},0) = c_0(\mathbf{x}) \qquad \text{for all } \mathbf{x} \in D \tag{27a}$$

$$s(\mathbf{x},0) = s_0(\mathbf{x}) \qquad \text{for all } \mathbf{x} \in D. \tag{27b}$$

The integral of equation (24) represents a generic management objective which can be defined specifically when the aquifer manager determines a particular goal for the cleanup project. In general, it is reasonable to assume that any management objective would depend on time, the pumping rate of the extraction well Q(t) [L^3/T], the contaminant concentration at the well, and the rate at which the concentration is changing at the well on a specified time interval. For example, one such management objective might be to minimize the volume of water pumped while maximizing the contaminant mass removed over a given period of time.

The functional in equation (24) is defined as a definite integral over a specific time interval [0, t_f] and around the *boundary* of the well. Treating the well as a boundary, subject to the boundary condition in (26a), introduces a point sink at the location of the well as the *boundary* of the well shrinks to a point. This approach was used to avoid introducing a generalized function (Dirac delta function) as a point sink in equation (16). In two dimensions, this boundary integral becomes the line integral around Γ_1:

$$\int_{B_w} f \, dB_w = \int_{\Gamma_1} f \, ds_1 , \tag{28}$$

and in three dimensions it becomes the surface integral around S_1:

$$\int_{B_w} f \, dB_w = \iint_{S_1} f \, dS_1 , \tag{29}$$

where Γ_1 is the circle defined by the perimeter of the well shaft in two dimensions, and S_1 is the surface of the cylinder of the screen at the end of the shaft in three dimensions, as shown in Figures 4 and 5.

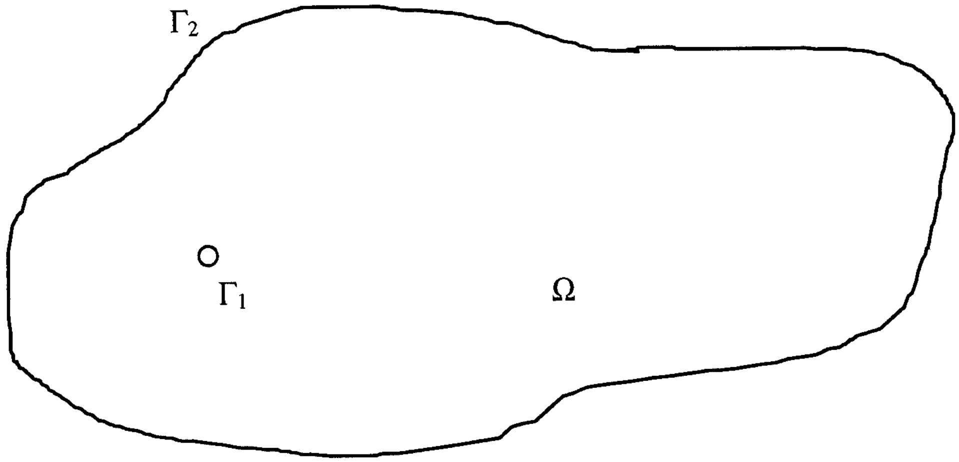

Figure 4. Two-Dimensional aquifer domain Ω with well *boundary* Γ_1 and domain boundary Γ_2.

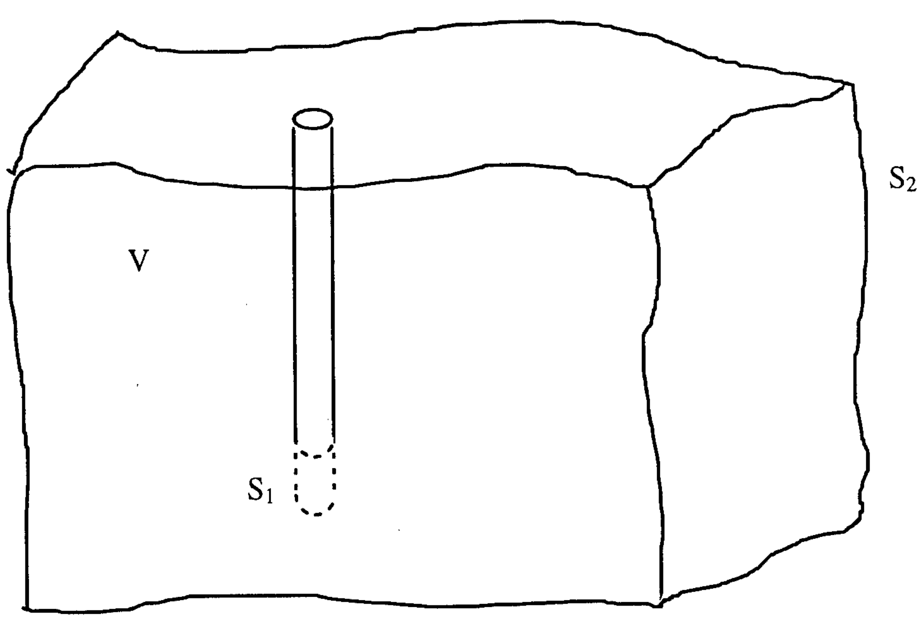

Figure 5. Three-Dimensional aquifer domain V with well *boundary* S_1 and domain boundary S_2.

Equations (24) through (28) define the optimization problem examined in this research. The next section develops an optimization approach that, when applied to these equations, leads to necessary and sufficient conditions for a minimum of the functional defined by (24).

3.4 *Variational Approach*

The classical calculus of variations approach (Gelfand & Fomin, 1963; Sagan, 1969) will determine an optimal pumping schedule by applying the first and second variations to the Lagrangian of the optimization problem given in section 3.3, where the Lagrangian is a single functional that combines the objective functional with the constraining equations. A number of the pertinent definitions and theorems of the calculus of variations are given here and are referenced throughout the analysis of the Lagrangian presented in Chapters IV through VII.

Examination of the so-called 'simplest' variational problem illustrates the concepts of the study of variational problems:

> Let F(x, y, z) be a function with continuous first and second partial derivatives with respect to all of its arguments. Then, among all functions y(x) which are continuously differentiable for $a \le x \le b$ and satisfy the boundary conditions
>
> $$y(a) = A, \qquad y(b) = B, \tag{30}$$
>
> find the function $\hat{y}(x)$ for which the functional
>
> $$J[y] = \int_a^b F(x, y, y')dx \tag{31}$$
>
> has a weak extremum (Gelfand & Fomin, 1963:14).

The functional J[y] has an extremum for $y = \hat{y}$ if $J[y] - J[\hat{y}]$ does not change sign in some neighborhood of the curve $y = \hat{y}(x)$. Additionally, J[y] has a *weak extremum* if there exists an $\varepsilon > 0$ such that $J[y] - J[\hat{y}]$ has the same sign for all y in the domain of the functional which satisfy the condition $\|y - \hat{y}\|_1 < \varepsilon$, where $\|*\|_1$ denotes the norm in the space $C^1([a, b])$ (the space of continuous functions with continuous first derivatives on [a, b]), given as

$$\|y\|_1 = \max_{a \le x \le b}|y(x)| + \max_{a \le x \le b}|y'(x)|.$$

Similarly, J[y} has a *strong extremum* if there exists an $\varepsilon > 0$ such that $J[y] - J[\hat{y}]$ has the same sign for all y in the domain of the functional which satisfy the condition $\|y - \hat{y}\|_0 < \varepsilon$, where $\|*\|_0$ denotes the norm in the space C([a, b]) (the space of continuous functions on [a, b]), given as

$$\|y\|_0 = \max_{a \le x \le b}|y(x)|.$$

The simplest problem can be modified in a number of ways, resulting in a much more challenging problem. For example, the boundary conditions in (30) might be made arbitrary, or y in the argument list of F might be a vector or might depend on more than one variable, or possibly the functional in (31) might have subsidiary conditions (constraints) imposed on the admissible curves, $\hat{y}(x)$. To find an extremum for a functional of the form of (31), we must first define the concept of the *first variation.*

Definition 1. Let J be a functional with $\mathcal{D}om(J) \subset \mathcal{R}$, a normed linear space over **R**, the set of reals. Let $y \in \mathcal{D}om(J)$ and h be arbitrary in $\mathcal{R}$. If the limit, where $\alpha \in \mathbf{R}$,

$$\delta J[y;h] = \lim_{\alpha \to 0} \frac{d}{d\alpha} J[y + \alpha h]$$

exists for all h, it is called the *first variation* of J at y with increment h (Sagan, 1969:26).

Another important idea is the so-called *set of admissible variations*. Recall, the simplest variational problem seeks to find an extremum $\hat{y}$, of a given functional, subject to specified boundary conditions. Thus, we are not interested in all $y \in C^1([a, b])$ but only those which satisfy the boundary conditions. The set of all functions from $C^1([a, b])$ which also satisfy the prescribed boundary conditions is called the *set of competing functions*, denoted by Σ. This leads to the following definition:

Definition 2. For a given space of competing functions $\Sigma \subset \mathcal{R}$, $H \subset \mathcal{R}$ is called a *set of admissible variations* of Σ if, for all $y \in \Sigma$, $h \in H$, $y + h \in \Sigma$ (Sagan, 1969:31).

Basically, $h \in H$ if y + h satisfies the prescribed boundary conditions on y. With these definitions, the first theorem which leads to necessary conditions for the existence of extrema is:

Theorem 1. A necessary condition for the differentiable functional J[y] to have an extremum for $y = \hat{y} \in \Sigma$ is that its first variation vanish for $y = \hat{y}$, that is

$$\delta J[\hat{y};h] = 0$$

for all variations $h \in H$ (Gelfand & Fomin, 1963:13).

In the case of the simplest variational problem, this theorem leads to a second-order differential equation known as Euler's equation which must be satisfied by an extremum. However, for the problem considered in this research, the function y above denotes the contaminant concentration in a confined aquifer at a particular observation point. The concentration levels within the aquifer are determined by the BVP presented in the preceding section as the constraints, or finite subsidiary conditions. For constrained problems, the following theorem applies.

Theorem 2. Given the functional

$$J[y,z] = \int_a^b F(x,y,z,y',z')dx \tag{32}$$

let the admissible curves (i.e., elements of Σ) lie on the surface

$$g(x,y,z) = 0 \tag{33}$$

and satisfy the boundary conditions

$$\begin{aligned} y(a) &= A_1, \qquad & y(b) &= B_1 \\ z(a) &= A_2, \qquad & z(b) &= B_2 \end{aligned} \tag{34}$$

and moreover, let J[y, z] have an extremum for the curve

$$y = y(x), \qquad\qquad z = z(x). \tag{35}$$

Then, if g_y and g_z do not vanish simultaneously at any point of the surface (33), there exists a function $\lambda(x)$ such that (35) is an extremal of the functional

$$\mathcal{L}[y,z,\lambda] = \int_a^b [F + \lambda(x)g]dx \tag{36}$$

(Gelfand & Fomin, 1963:46).

Equation (36) is called the Lagrangian for the optimization problem defined by the objective functional in (32) and the constraint defined by (33). Theorem 2 states that the given objective functional has an optimal solution on the same curve as the optimal solution of the Lagrangian. Thus, if the Lagrangian in (36) is optimized, then so is the objective functional in (32) and necessary optimality conditions (NOCs) are found by applying Theorem 1 to the Lagrangian in (36).

For the optimization problem of section 3.3, the Lagrangian is given as

$$\begin{aligned}\mathcal{L}[Q,c,\lambda] &= \int_0^{t_f}\int_{B_w} f(t,Q(t),c(\mathbf{x},t),c_t(\mathbf{x},t))\,dB_w\,dt \\ &+ \int_0^{t_f}\int_D \lambda(\mathbf{x},t)\left\{\begin{aligned}&L[c(\mathbf{x},t)]+\frac{\rho_B\alpha}{\theta}e^{-\alpha t}s_0(\mathbf{x})-c_t(\mathbf{x},t)\\ &+\frac{\rho_B\alpha^2K_d}{\theta}e^{-\alpha t}\int_0^t c(\mathbf{x},\tau)e^{\alpha\tau}d\tau\end{aligned}\right\}dxdt,\end{aligned} \tag{37}$$

where the operator L is defined as

$$L[c]=\nabla\cdot(\underline{\underline{D}}_h\cdot\nabla c)-\nabla\cdot(vc)-\frac{\rho_B\alpha K_d}{\theta}c. \tag{38}$$

The region of integration D in (37) is defined by the domain (Ω in two dimensions, V in three dimensions) of the confined aquifer, and the function $\lambda(\mathbf{x},t)$ is called the Lagrange multiplier introduced in Theorem 2. Chapter IV of this document investigates the first variation of the Lagrangian in (37) to derive NOCs for an extremum. More NOCs and sufficient optimality conditions (SOCs) are derived by investigating the *second variation* of the Lagrangian, defined as follows:

Definition 3. Let J be a functional with $\mathcal{D}om(J) \subset \mathcal{R}$, a normed linear space over **R**. Let $y \in \mathcal{D}om(J)$ and h be arbitrary in $\mathcal{R}$. If the limit, where $\alpha \in \mathbf{R}$

$$\delta^2 J[y;h] = \frac{1}{2}\lim_{\alpha \to 0}\frac{d^2}{d\alpha^2}J[y+\alpha h]$$

exists for all $h \in \mathcal{R}$, it is called the *second variation* of J at y with increment h (Sagan, 1969:35).

In applying Definition 3, we find that the second variation turns out to be a *quadratic functional* (Note, a functional B[x,y] depending on two elements x and y, belonging to some normed linear space $\mathcal{R}$, is said to be *bilinear* if it is a linear functional of y for any fixed x and a linear functional of x for any fixed y. That is,

$$\begin{aligned} B[x+z,y] &= B[x,y]+B[z,y] \\ B[\alpha x,y] &= \alpha B[x,y] \end{aligned}$$

and

$$\begin{aligned} B[x,y+z] &= B[x,y]+B[x,z] \\ B[x,\alpha y] &= \alpha B[x,y] \end{aligned}$$

for any x, y, $z \in \mathcal{R}$ and $\alpha \in \mathbf{R}$. If we set y = x in a bilinear functional, we obtain a *quadratic functional* (Gelfand & Fomin, 1963:97).). Also, note that a quadratic functional $\varphi[h]$, defined on some normed linear space, is said to be *strongly positive* if there exists a constant $k > 0$ such that $\varphi[h] \geq k\|h\|^2$ for all h. In a finite dimensional space, strong positivity of a quadratic functional is equivalent to positive definiteness but, in general, strong positivity is a stronger condition than positive definiteness. The next two theorems provide the basis for the work presented in Chapters V and VI.

Theorem 3. Given that $\delta J[\hat{y}; h] = 0$ for all admissible variations, h, a necessary condition for the functional J[y] to have a minimum for $y = \hat{y} \in \Sigma$ is that

$$\delta^2 J[\hat{y}; h] \geq 0$$

for all admissible variations, h. For a maximum, the sign $\geq$ is replaced by $\leq$ (Gelfand & Fomin, 1963:99).

Theorem 4. A sufficient condition for a functional J[y] to have a minimum for $y = \hat{y}$, given that the first variation $\delta J[y; h]$ vanishes for $y = \hat{y}$, is that its second variation $\delta^2 J[y; h]$ be strongly positive for $y = \hat{y}$ (Gelfand & Fomin, 1963:100).

In Chapter V, the second variation of the Lagrangian in (37) is presented and Theorem 3 provided the basis for the analysis that led to necessary optimality conditions for the second variation. Theorem 4 justifies the work in Chapter VI, where sufficiency conditions for a minimum solution are found. Chapter VI establishes conditions on the positive definiteness of the second variation found in Chapter V, thus providing sufficient optimality conditions for a minimum stated in the form of a theorem at the end of Chapter VI.

3.5 Summary

The analysis performed in this research pursues the theory presented in the preceding section. The first and second variations of the Lagrangian presented in (37) lead to NOCs and SOCs that establish an optimal pulsed pumping schedule. The next four chapters of this document derive these NOCs and SOCs, demonstrate how to use

them to establish an optimal pulsed pumping schedule, and examine general classes of functionals, establishing conditions to determine what types of objectives can be optimized with a pulsed pumping approach.

The purpose of the present chapter was to establish the mathematical foundation for the material that follows in the rest of this document. The next chapter presents the full investigation of the first variation of the Lagrangian, given by equation (37). The time interval defined by the objective functional was divided into n intervals of on/off pumping periods (Figure 3). The first variation of the Lagrangian on the ith interval was then examined and Theorem 1 was applied for all admissible variations of each of the independent variables, leading to NOCs for the first variation. These NOCs provided a tool to find a candidate optimal pumping schedule, consisting of pump on/off switching times, for the optimization problem in 3.3. Using this candidate solution, necessary conditions for the optimal solution to produce a minimum for the functional in (24) were determined by applying the theorems related to the second variation of the Lagrangian. The second variation was found through the use of Definition 3, and its derivation is presented in Chapter V. Additionally, Chapter V presents the application of Theorem 3 which led to necessary conditions (for the second variation of the Lagrangian) for the optimal pumping schedule to produce a minimum for the functional (24). The work presented in Chapter VI culminates with a theorem that provides both necessary and sufficient conditions for the existence of a minimum. Motivated by Theorem 4, SOCs for the optimization problem were derived that guaranteed the optimal pumping schedule found in Chapter IV provided a solution that minimized (24). Finally, this technique was

applied to general classes of functionals, and specific examples that illustrate the technique are presented in Chapter VII.

IV. Necessary Optimality Conditions of the First Variation

The preceding chapters of this dissertation have discussed the general problem of groundwater remediation, previous investigations of optimal management and design of pump-and-treat facilities, and finally an analytical optimization method that was applied in the work described here. This chapter presents an examination of the first variation of the Lagrangian defined by (37). Application of Theorems 1 and 2 of Chapter III led to necessary optimality conditions (NOCs) for an optimal pulsed pumping schedule, and their derivations are presented here in the proof of a necessary conditions theorem. These NOCs provide a candidate pulsed pumping schedule, dependent upon the selection of an objective functional that describes a particular goal, as determined by a remediation site manager. Subsequent investigation of the second variation determined necessary and sufficient conditions that this optimal pumping schedule yields a minimum solution for the given optimization problem.

4.1 First Variation of the Lagrangian

In this section, we derive the first variation of the Lagrangian in two dimensions. The derivation in three dimensions is similar and will not be presented here. The Lagrangian in two dimensions (**x** is the point (x,y) and d**x** = dxdy) is given as

$$\begin{aligned}\mathcal{L}[Q,c,\lambda] &= \int_0^{t_f}\int_{\Gamma_1} f(t,Q(t),c(s,t),c_t(s,t))\,ds_1dt \\ &+ \int_0^{t_f}\int_\Omega \lambda(\mathbf{x},t)\left\{[Lc](\mathbf{x},t) + \frac{\rho_B\alpha}{\theta}e^{-\alpha t}s_0(\mathbf{x}) - c_t(\mathbf{x},t) + \frac{\rho_B\alpha^2K_d}{\theta}e^{-\alpha t}\int_0^t c(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right\}d\mathbf{x}dt,\end{aligned} \tag{39}$$

where the operator L is defined in (38) and the parametric equations of Γ are introduced as $x = x(s)$ and $y = y(s)$, where s is the parameter. Thus, $c(s,t)$ means $c(x(s), y(s), t) = c(\mathbf{x}(s),t)$ and "the point s" means the point $(x(s), y(s))$, and integrating around Γ_1 means to integrate over the arc length of the extraction well, given as $|\Gamma_1| = 2\pi r_w$, where r_w is the radius of the extraction well. The time interval $[0, t_f]$ has n distinct intervals where the pump is either on or off, as depicted in figure 3. In this research, the pump was assumed to be on initially and on during the last interval, implying that n is an odd number and the pump is off during even numbered intervals and on during odd numbered intervals.

The Lagrangian in (39) is a functional of three variables. In finding the first variation of (39), each of these variables will be allowed to vary as described in Definition 1. Careful manipulation of the Lagrangian led to a decision to reverse the order of integration on $d\tau dt$. This allowed the first variation of the Lagrangian to (eventually) be written as a sum of the variations with respect to each of the variables Q, c, and λ, independently. Thus, equation (39) can be rewritten as

$$\begin{aligned}\mathcal{L}[Q,c,\lambda] = {} & \int_0^{t_f}\int_{\Gamma_1} f(t,Q(t),c(s,t),c_t(s,t))ds_1 dt \\ & + \int_0^{t_f}\int_\Omega \left\{ \begin{aligned} & \lambda(\mathbf{x},t)\left[[Lc](\mathbf{x},t) + \frac{\rho_B\alpha}{\theta}e^{-\alpha t}s_0(\mathbf{x}) - c_t(\mathbf{x},t)\right] \\ & + \frac{\rho_B\alpha^2 K_d}{\theta}e^{\alpha t}c(\mathbf{x},t)\int_t^{t_f}\lambda(\mathbf{x},\tau)e^{-\alpha\tau}d\tau \end{aligned} \right\} d\mathbf{x}dt. \end{aligned} \tag{40}$$

Note also, the variation of the Lagrangian in (40) is equal to the sum of the variations of the Lagrangians defined on each of the intervals in Figure 3. That is,

$$\delta\mathcal{L}[Q,c,\lambda] = \sum_{i=1}^{n}\delta\mathcal{L}^{(i)}[Q^{(i)},c^{(i)},\lambda^{(i)}], \tag{41}$$

where

$$\mathcal{L}^{(i)}[Q^{(i)},c^{(i)},\lambda^{(i)}] = \int_{t_{i-1}}^{t_i}\int_{\Gamma_1} f(t,Q^{(i)}(t),c^{(i)}(s,t),c_t^{(i)}(s,t))ds_1dt + \int_{t_{i-1}}^{t_i}\int_{\Omega}\left\{\begin{aligned}&\lambda^{(i)}(\mathbf{x},t)\big([L^{(i)}c^{(i)}](\mathbf{x},t)+a_0(\mathbf{x},t)-c_t^{(i)}(\mathbf{x},t)\big)\\ &+Ae^{\alpha t}c^{(i)}(\mathbf{x},t)\int_t^{t_f}\lambda(\mathbf{x},\tau)e^{-\alpha\tau}d\tau\end{aligned}\right\}d\mathbf{x}dt. \tag{42}$$

In equations (41) and (42), the pumping schedule is defined as

$$Q^{(i)}(t) = \begin{cases} Q_{ON} & \text{for i odd} \\ 0 & \text{for i even} \end{cases} \tag{43}$$

for all $t \in [0, t_f]$, where Q_{ON} is a predetermined, constant pumping rate and the spatial differential operators are defined as

$$L^{(i)} = \begin{cases} L^{ON} & \text{for i odd} \\ L^{OFF} & \text{for i even} \end{cases} \tag{44}$$

where the operators L^{ON} and L^{OFF} defined by (38) and (18) change on each interval, depending on the status of the pump. Additionally, $c^{(i)}(\mathbf{x},t)$ and $\lambda^{(i)}(\mathbf{x},t)$ are defined as the concentration and the Lagrange multiplier for the i^{th} interval, $[t_{i-1}, t_i]$, where $t_0 = 0$ and $t_n = t_f$. Finally, the known quantities $a_0(\mathbf{x},t)$ and A are defined as

$$a_0(\mathbf{x},t) = \frac{\rho_B\alpha}{\theta}e^{-\alpha t}s_0(\mathbf{x}) \tag{45}$$

and

$$A = \frac{\rho_B\alpha^2K_d}{\theta}, \tag{46}$$

which do not dependent on Q, c, or λ.

Applying Definition 1 to the Lagrangian in the i^{th} interval and suppressing the superscript (i) for notational convenience, the variation could be written as

$$\delta\mathcal{L}[Q,c,\lambda;K,h,\mu] = \lim_{a\to 0}\frac{\partial}{\partial a}\mathcal{L}[Q+aK,c+ah,\lambda+a\mu], \tag{47}$$

where K, h, and μ are the variations of Q, c, and λ, respectively. However, the pumping rate, Q is an element of the set S, (S is stated immediately following equation (1) where $Q_{max} = Q_{ON}$), which represents the set of competing functions for optimal Q. Recalling the comment after Definition 2, we see that Q + K certainly would not satisfy boundary conditions on constant Q(t) at the endpoints t_{i-1} and t_i. Thus, Q + aK does not make sense in (47). Additionally, we do not seek to find an optimal pumping rate, but rather optimal times to switch from pumping at a constant rate to not pumping at all, continually repeating the process. So, the variation of the functional in (42) due to Q(t) is not dependent on the pumping rate, but rather the switching times t_{i-1} and t_i. Thus, the first variation of (42) can be written more precisely as

$$\begin{aligned}\delta\mathcal{L}^{(i)}[Q^{(i)},c^{(i)},\lambda^{(i)}] &= \delta\mathcal{L}^{(i)}[t_{i-1},t_i,c^{(i)},\lambda^{(i)};\Delta t_{i-1},\Delta t_i,h^{(i)},\mu^{(i)}]\\ &= \lim_{a\to 0}\frac{\partial}{\partial a}\mathcal{L}^{(i)}[t_{i-1}+a\Delta t_{i-1},t_i+a\Delta t_i,c^{(i)}+ah^{(i)},\lambda^{(i)}+a\mu^{(i)}],\end{aligned} \tag{48}$$

where Δt_{i-1} and Δt_i are the variations of the endpoints of the i^{th} interval. Before applying (48) to (42), we simplify the presentation by defining the one parameter families of functions $\Lambda^{(i)}(\mathbf{x},t;a)$ and $C^{(i)}(\mathbf{x},t;a)$, where $t \in [t_{i-1}, t_i]$, such that for each i = 1, 2, ... n

$$\Lambda^{(i)}(\mathbf{x},t;a) = \lambda^{(i)}(\mathbf{x},t) + a\mu^{(i)}(\mathbf{x},t), \quad \text{which implies that} \quad \begin{cases} \Lambda^{(i)}(\mathbf{x},t;0) = \lambda^{(i)}(\mathbf{x},t) \\ \Lambda^{(i)}_a(\mathbf{x},t;0) = \mu^{(i)}(\mathbf{x},t), \\ \Lambda^{(i)}_{aa}(\mathbf{x},t;0) = 0 \end{cases} \tag{49a}$$

and

$$C^{(i)}(\mathbf{x},t;a) = c^{(i)}(\mathbf{x},t) + ah^{(i)}(\mathbf{x},t), \quad \text{which implies that} \quad \begin{cases} C^{(i)}(\mathbf{x},t;0) = c^{(i)}(\mathbf{x},t) \\ C^{(i)}_a(\mathbf{x},t;0) = h^{(i)}(\mathbf{x},t), \\ C^{(i)}_{aa}(\mathbf{x},t;0) = 0 \end{cases} \tag{49b}$$

and also defining $T^{(i)}(a)$ for all i = 0, 1, ... n, such that

$$T^{(i)}(a) = t_i + a\Delta t_i, \quad \text{which implies that} \quad \begin{cases} T^{(i)}(0) = t_i \\ T^{(i)}_a(0) = \Delta t_i \\ T^{(i)}_{aa}(0) = 0 \end{cases} \tag{49c}$$

where subscript a denotes the partial derivative with respect to a. Thus, we can write (48) in a more compact form as

$$\delta\mathcal{L}^{(i)}[Q^{(i)},c^{(i)},\lambda^{(i)}] = \lim_{a\to 0}\frac{\partial}{\partial a}\mathcal{L}^{(i)}[T^{(i-1)}(a),T^{(i)}(a),C^{(i)}(\mathbf{x},t;a),\Lambda^{(i)}(\mathbf{x},t;a)]. \tag{50}$$

Equation (50) characterized the first variation of the Lagrangian on the i^{th} interval, and this form was applied to equation (42). Suppressing the arguments of the functions $Q^{(i)}$, $C^{(i)}$, $\Lambda^{(i)}$, and $T^{(i)}$, and the superscripts on $C^{(i)}$ and $\Lambda^{(i)}$ (except when more than one interval is considered) we have

$$\begin{aligned} \delta\mathcal{L}^{(i)}[Q^{(i)},c^{(i)},\lambda^{(i)}] = \lim_{a\to 0}\frac{\partial}{\partial a}\Big\{ & \int_{T^{(i-1)}}^{T^{(i)}}\int_{\Gamma_1} f(t,Q^{(i)},C,C_t)ds_1dt \\ & + \int_{T^{(i-1)}}^{T^{(i)}}\int_{\Omega}\Big(\Lambda\big[L^{(i)}C - C_t + a_0\big] + Ae^{\alpha t}C\int_t^{t_f}\Lambda(\mathbf{x},\tau;a)e^{-\alpha\tau}d\tau\Big)d\mathbf{x}dt\Big\}. \end{aligned} \tag{51}$$

Notice, in (51) that the integral inside the second term can be written as

$$\int_t^{t_f} \Lambda(\mathbf{x},\tau;a)e^{-\alpha\tau}d\tau = \int_t^{T^{(i)}} \Lambda^{(i)}(\mathbf{x},\tau;a)e^{-\alpha\tau}d\tau + \cdots + \int_{T^{(n-1)}}^{t_f} \Lambda^{(n)}(\mathbf{x},\tau;a)e^{-\alpha\tau}d\tau, \qquad (52)$$

where the superscript on Λ indicates the interval and i depends on t. To take the derivative (with respect to the parameter a) of the expression contained in (51) and (52), Leibnitz's rule will be used.

Theorem 5. (Leibnitz's rule) Assume $f : \mathbf{R} \times [a, b] \to \mathbf{R}$ and $f(t,\alpha)$ and $\partial f/\partial\alpha$ are both continuous on $\mathbf{R} \times [a, b]$. Also, assume $u_1, u_2 : \mathbf{R} \to \mathbf{R}$ are continuous and have continuous derivatives for $a \le \alpha \le b$. Define

$$G(\alpha) = \int_{u_1(\alpha)}^{u_2(\alpha)} f(t,\alpha)dt \qquad a \le \alpha \le b.$$

Then

$$\frac{\partial G(\alpha)}{\partial\alpha} = \int_{u_1(\alpha)}^{u_2(\alpha)} \frac{\partial f(t,\alpha)}{\partial\alpha}dt + f(u_2(\alpha),\alpha)\frac{\partial u_2(\alpha)}{\partial\alpha} - f(u_1(\alpha),\alpha)\frac{\partial u_1(\alpha)}{\partial\alpha}$$

for $a < \alpha < b$ (Spiegel, 1963:163).

Using Leibnitz's rule in (51) and (52) and suppressing argument variables when it is clear, yields

$$\delta\mathcal{L}^{(i)}[Q^{(i)},c^{(i)},\lambda^{(i)}] = \lim_{a\to 0}\left\{\int_{T^{(i-1)}}^{T^{(i)}}\int_{\Gamma_1}(f_c C_a + f_{c_t} C_{ta})ds_1 dt + \int_{\Gamma_1} f\Big|_{t=T^{(i)}} ds_1 T_a^{(i)} - \int_{\Gamma_1} f\Big|_{t=T^{(i-1)}} ds_1 T_a^{(i-1)}\right.$$
$$\left. + \int_{T^{(i-1)}}^{T^{(i)}}\int_{\Omega}\left\{\begin{array}{l} \Lambda_a\left[L^{(i)}C - C_t + a_0\right] + \Lambda\left[L^{(i)}C_a - C_{ta}\right] + AC_a e^{\alpha t}\int_t^{t_f}\Lambda(\mathbf{x},\tau;a)e^{-\alpha\tau}d\tau \\ +ACe^{\alpha t}\left\{\int_t^{t_f}\Lambda(\mathbf{x},\tau;a)e^{-\alpha\tau}d\tau + \Lambda^{(i)}(\mathbf{x},T^{(i)}(a);a)e^{-\alpha T^{(i)}}T_a^{(i)} + \cdots\right. \\ \qquad \left.\cdots - \Lambda^{(n)}(\mathbf{x},T^{(n-1)}(a);a)e^{-\alpha T^{(n-1)}}T_a^{(n-1)}\right\} \end{array}\right\}dxdt\right.$$

$$
\begin{aligned}
&+\int_\Omega \Big(\Lambda\big[L^{(i)}C - C_t + a_0\big]\Big|_{t=T^{(i)}} + ACe^{\alpha T^{(i)}}\int_{T^{(i)}}^{t_f}\Lambda(\mathbf{x},\tau;a)e^{-\alpha\tau}d\tau\Big)d\mathbf{x}T_a^{(i)} \\
&-\int_\Omega \Big(\Lambda\big[L^{(i)}C - C_t + a_0\big]\Big|_{t=T^{(i-1)}} + ACe^{\alpha T^{(i-1)}}\int_{T^{(i-1)}}^{t_f}\Lambda(\mathbf{x},\tau;a)e^{-\alpha\tau}d\tau\Big)d\mathbf{x}T_a^{(i-1)}\Big\}.
\end{aligned} \tag{53}
$$

As in the classical approach to the variational problem, we integrate by parts (over t) on all terms above which include C_t. In order to do this, we assume that the integral is continuous on the i^{th} interval, and we have

$$
\int_{T^{(i-1)}}^{T^{(i)}}\int_{\Gamma_1} f_{c_t} C_{ta}\, ds_1 dt = \int_{\Gamma_1} f_{c_t} C_a\Big|_{t=T^{(i-1)}}^{t=T^{(i)}} ds_1 - \int_{T^{(i-1)}}^{T^{(i)}}\int_{\Gamma_1} C_a \frac{\partial}{\partial t} f_{c_t}\, ds_1 dt \tag{54a}
$$

and

$$
\begin{aligned}
\int_{T^{(i-1)}}^{T^{(i)}}\int_\Omega(-C_t\Lambda_a - C_{ta}\Lambda)d\mathbf{x}dt = -\int_\Omega C\Lambda_a\Big|_{t=T^{(i-1)}}^{t=T^{(i)}} d\mathbf{x} - \int_\Omega C_a\Lambda\Big|_{t=T^{(i-1)}}^{t=T^{(i)}} d\mathbf{x} \\
+\int_{T^{(i-1)}}^{T^{(i)}}\int_\Omega (C\Lambda_{at} + C_a\Lambda_t)d\mathbf{x}dt.
\end{aligned} \tag{54b}
$$

The integration by parts above was performed in order to introduce *time* boundary terms for the i^{th} interval. Essentially, on the i^{th} interval the endpoints of the curves for which (40) is defined can move in an arbitrary way. Thus, we must use caution when dealing with C and Λ at the points $T^{(i)}$ for all i = 0, 1, ... n. With this in mind, define

$$
\mathcal{C}^{(i)}(\mathbf{x},a) = C(\mathbf{x},T^{(i)}(a);a) \qquad \text{and} \qquad \Psi^{(i)}(\mathbf{x},a) = \Lambda(\mathbf{x},T^{(i)}(a);a) \tag{55}
$$

then

$$
\mathcal{C}_a^{(i)} = C_t T_a^{(i)} + C_a \qquad \text{and} \qquad \Psi_a^{(i)} = \Lambda_t T_a^{(i)} + \Lambda_a. \tag{56}
$$

Also, note that

$$
T_a^{(0)}(a) = T_a^{(n)}(a) = 0,
$$

since the endpoints of the entire interval are fixed ($t_0 = 0$ and $t_n = t_f$ implies $\Delta t_0 = \Delta t_n = 0$). Finally, we define the variations

$$\delta c_i(\mathbf{x}) = \lim_{a\to 0} \mathcal{C}_a^{(i)}(\mathbf{x},a) \qquad \text{and} \qquad \delta\lambda_i(\mathbf{x}) = \lim_{a\to 0} \Psi_a^{(i)}(\mathbf{x},a), \tag{57}$$

where $\delta c_i(\mathbf{x})$ and $\delta\lambda_i(\mathbf{x})$ are the variations of $c(\mathbf{x},t)$ and $\lambda(\mathbf{x},t)$, respectively, due to the variable endpoints, t_i. From (56) and (57), note that

$$\left.\begin{aligned} h(\mathbf{x},t_i) &= \delta c(\mathbf{x})_i - c_t(\mathbf{x},t_i)\Delta t_i \\ \mu(\mathbf{x},t_i) &= \delta\lambda(\mathbf{x})_i - \lambda_t(\mathbf{x},t_i)\Delta t_i \end{aligned}\right\} \text{ for each } i = 0,\ 1,\ \ldots\ n. \tag{58}$$

Also, since t_0 and t_n are fixed, then $\delta c_0(\mathbf{x}) = h(\mathbf{x}, 0)$, $\delta c_n(\mathbf{x}) = h(\mathbf{x}, t_f)$, $\delta\lambda_0(\mathbf{x}) = \mu(\mathbf{x}, 0)$, and $\delta\lambda_n(\mathbf{x}) = \mu(\mathbf{x}, t_f)$. Now, introducing (54) - (57), into (53), letting $a \to 0$ (note that all functions change to lower case due to definitions in (49)) leaves

$$\begin{aligned}
\delta\mathcal{L}^{(i)}[Q^{(i)}, c^{(i)}, \lambda^{(i)}] &= \int_{t_{i-1}}^{t_i}\int_{\Gamma_1}(f_c - \frac{\partial}{\partial t} f_{c_t})h(s,t)\,ds_1 dt \\
&+ \int_{\Gamma_1}\left([f_{c_t}\delta c_i + (f - f_{c_t}c_t)\Delta t_i]\Big|_{t=t_i} - [f_{c_t}\delta c_{i-1} + (f - f_{c_t}c_t)\Delta t_{i-1}]\Big|_{t=t_{i-1}}\right)ds_1 \\
&+ \int_{t_{i-1}}^{t_i}\int_{\Omega}\left(\begin{aligned} &\mu_t c + \mu[L^{(i)}c + a_0] + Ace^{\alpha t}\Big\{\int_t^{t_f}\mu(\mathbf{x},\tau)e^{-\alpha\tau}d\tau + \lambda^{(i)}e^{-\alpha t}\Big|_{t=t_i}\Delta t_i + \cdots \\ &\cdots - \lambda^{(n)}e^{-\alpha t}\Big|_{t=t_{n-1}}\Delta t_{n-1}\Big\} + \lambda_t h + \lambda L^{(i)}h + Ahe^{\alpha t}\int_t^{t_f}\lambda(\mathbf{x},\tau)e^{-\alpha\tau}d\tau \end{aligned}\right)dxdt \\
&- \int_{\Omega}\left(\begin{aligned} &[c(\delta\lambda_i - \lambda_t\Delta t_i) + \lambda(\delta c_i - c_t\Delta t_i) - \lambda(L^{(i)}c - c_t + a_0)\Delta t_i]\Big|_{t=t_i} \\ &-[c(\delta\lambda_{i-1} - \lambda_t\Delta t_{i-1}) + \lambda(\delta c_{i-1} - c_t\Delta t_{i-1}) - \lambda(L^{(i)}c - c_t + a_0)\Delta t_{i-1}]\Big|_{t=t_{i-1}} \\ &- Ac(\mathbf{x},t_i)e^{\alpha t_i}\int_{t_i}^{t_f}\lambda(\mathbf{x},\tau)e^{-\alpha\tau}d\tau\Delta t_i + Ac(\mathbf{x},t_{i-1})e^{\alpha t_{i-1}}\int_{t_{i-1}}^{t_f}\lambda(\mathbf{x},\tau)e^{-\alpha\tau}d\tau\Delta t_{i-1} \end{aligned}\right)d\mathbf{x}.
\end{aligned} \tag{59}$$

Equation (59) is the first variation of the Lagrangian on the i^{th} interval. In the next section of this chapter, we examine the first variation of the Lagrangian for all admissible values of the variations h, μ, Δt_i, δc_i and $\delta\lambda_i$. The analysis presented in the next section is easier to follow if each of the integral terms in (59) is written in the form of an inner product between the variation and the differential operators. With this in mind, we manipulate the spatial derivative terms. Recall the operator $L^{(i)}$ is defined as

$$L^{(i)}[c] = \nabla \cdot (\underline{\underline{D}}_h^{(i)} \cdot \nabla c) - \nabla \cdot (\mathbf{v}^{(i)} c) - \frac{\rho_B \alpha K_d}{\theta} c, \tag{60}$$

where the superscripts on the right-hand side denote the terms that depend on the status of the pump. Through use of the divergence theorem, we derive the identity

$$\int_\Omega \lambda L^{(i)} c d\mathbf{x} = \int_\Omega c L^{*(i)} \lambda d\mathbf{x} + \int_\Gamma \left[\lambda(\underline{\underline{D}}_h^{(i)} \cdot \nabla c - c\mathbf{v}^{(i)}) - c\underline{\underline{D}}_h^{(i)} \cdot \nabla\lambda\right] \cdot \hat{\mathbf{n}} dsdt, \tag{61}$$

where the adjoint operator $L^{*(i)}$ is given by

$$L^{*(i)}[\lambda] = \nabla \cdot (\underline{\underline{D}}_h^{(i)} \cdot \nabla\lambda) + \mathbf{v}^{(i)} \cdot \nabla\lambda - \frac{\rho_B \alpha K_d}{\theta} \lambda, \tag{62}$$

and $\Gamma = \Gamma_1 \cup \Gamma_2$ is the boundary of the domain Ω (Figure 4) and $\hat{\mathbf{n}}$ is the unit outward normal to the boundary. With the boundary conditions defined by (20), the boundary integral in (61) becomes

$$\begin{aligned} &\int_\Gamma \left[\lambda(\underline{\underline{D}}_h^{(i)} \cdot \nabla c - c\mathbf{v}^{(i)}) - c\underline{\underline{D}}_h^{(i)} \cdot \nabla\lambda\right] \cdot \hat{\mathbf{n}} dsdt \\ &\quad = -\int_{\Gamma_2} c\underline{\underline{D}}_h^{(i)} \cdot \nabla\lambda \cdot \hat{\mathbf{n}}_2 ds_2 dt + \int_{\Gamma_1} \left[c(\underline{\underline{D}}_h^{(i)} \cdot \nabla\lambda + \lambda\mathbf{v}^{(i)})\right] \cdot \hat{\mathbf{n}}_1 ds_1 dt. \end{aligned} \tag{63}$$

The identity in (61) is now introduced into (59), but only where the adjoint will operate on the Lagrange multiplier λ. Also note, admissible h must satisfy the same homogeneous boundary conditions as the concentration. Thus, equations (61) and (63) could both be written with h substituted for c in both expressions. Finally, using these identities and with some cancellation and rearranging, (59) becomes

$$
\begin{aligned}
&\delta\mathcal{L}^{(i)}[Q^{(i)},c^{(i)},\lambda^{(i)}] \\
&\left.\begin{aligned}
&= \int_{t_{i-1}}^{t_i}\Big\{\int_{\Gamma_1}(f_c - \frac{\partial}{\partial t} f_{c_t})h(s,t)\,ds_1 \\
&\qquad + \int_\Omega h(\mathbf{x},t)\Big(L^{*(i)}\lambda + \lambda_t + Ae^{\alpha t}\int_t^{t_f}\lambda(\mathbf{x},\tau)e^{-\alpha\tau}d\tau\Big)\,d\mathbf{x} \\
&\qquad - \int_{\Gamma_2} h(s,t)\underline{\underline{D}}_h^{(i)}\cdot\nabla\lambda\cdot\hat{\mathbf{n}}_2\,ds_2 + \int_{\Gamma_1}\Big[h(s,t)(\underline{\underline{D}}_h^{(i)}\cdot\nabla\lambda+\lambda\mathbf{v}^{(i)})\Big]\cdot\hat{\mathbf{n}}_1\,ds_1\Big\}dt
\end{aligned}\right\} h^{(i)}\text{ terms} \\[2ex]
&\left.\begin{aligned}
&+\int_{t_{i-1}}^{t_i}\int_\Omega\Big(\mu_t c + \mu[L^{(i)}c + a_0] + Ace^{\alpha t}\Big\{\int_t^{t_f}\mu(\mathbf{x},\tau)e^{-\alpha\tau}d\tau + \lambda^{(i)}e^{-\alpha t}\Big|_{t=t_i}\Delta t_i + \cdots \\
&\qquad\qquad\qquad\qquad \cdots - \lambda^{(n)}e^{-\alpha t}\Big|_{t=t_{n-1}}\Delta t_{n-1}\Big\}\Big)\,d\mathbf{x}dt
\end{aligned}\right\} \mu^{(i)}\text{ terms} \\[2ex]
&\left.\begin{aligned}
&+\int_{\Gamma_1}[(f - f_{c_t}c_t)]\Big|_{t=t_i}\,ds_1\Delta t_i \\
&\qquad +\int_\Omega\Big\{[c(L^{*(i)}\lambda+\lambda_t)+\lambda a_0]\Big|_{t=t_i} + Ac(\mathbf{x},t_i)e^{\alpha t_i}\int_{t_i}^{t_f}\lambda(\mathbf{x},\tau)e^{-\alpha\tau}d\tau\Big\}\,d\mathbf{x}\Delta t_i \\
&\qquad -\int_{\Gamma_2} c\underline{\underline{D}}_h^{(i)}\cdot\nabla\lambda\Big|_{t=t_i}\cdot\hat{\mathbf{n}}_2\,ds_2\Delta t_i + \int_{\Gamma_1}\Big[c(\underline{\underline{D}}_h^{(i)}\cdot\nabla\lambda+\lambda\mathbf{v}^{(i)})\Big]\Big|_{t=t_i}\cdot\hat{\mathbf{n}}_1\,ds_1\Delta t_i
\end{aligned}\right\} \Delta t_i\text{ terms} \\[2ex]
&\left.\begin{aligned}
&-\int_{\Gamma_1}[(f - f_{c_t}c_t)]\Big|_{t=t_{i-1}}\,ds_1\Delta t_{i-1} \\
&\qquad -\int_\Omega\Big\{[c(L^{*(i)}\lambda+\lambda_t)+\lambda a_0]\Big|_{t=t_{i-1}} + Ac(\mathbf{x},t_{i-1})e^{\alpha t_{i-1}}\int_{t_{i-1}}^{t_f}\lambda(\mathbf{x},\tau)e^{-\alpha\tau}d\tau\Big\}\,d\mathbf{x}\Delta t_{i-1} \\
&\qquad +\int_{\Gamma_2} c\underline{\underline{D}}_h^{(i)}\cdot\nabla\lambda\Big|_{t=t_{i-1}}\cdot\hat{\mathbf{n}}_2\,ds_2\Delta t_{i-1} - \int_{\Gamma_1}\Big[c(\underline{\underline{D}}_h^{(i)}\cdot\nabla\lambda+\lambda\mathbf{v}^{(i)})\Big]\Big|_{t=t_{i-1}}\cdot\hat{\mathbf{n}}_1\,ds_1\Delta t_{i-1}
\end{aligned}\right\} \Delta t_{i-1}\text{ terms}
\end{aligned}
$$

$$+\int_{\Gamma_1} f_{c_t}\delta c_i\Big|_{t=t_i} ds_1 - \int_\Omega [c(\mathbf{x},t_i)\delta\lambda_i + \lambda(\mathbf{x},t_i)\delta c_i]d\mathbf{x} \quad \Big\}\ \delta c_i \text{ and } \delta\lambda_i \text{ terms}$$

$$(64)$$

$$-\int_{\Gamma_1} f_{c_t}\delta c_{i-1}\Big|_{t=t_{i-1}} ds_1 + \int_\Omega [c(\mathbf{x},t_{i-1})\delta\lambda_{i-1} + \lambda(\mathbf{x},t_{i-1})\delta c_{i-1}]d\mathbf{x}. \quad \Big\}\ \delta c_{i-1} \text{ and } \delta\lambda_{i-1} \text{ terms}$$

The equation in (64) represents the variation of the Lagrangian for any interval $i = 1, 2, \ldots n$, except for some minor changes for $i = 1$ and for $i = n$. That is, for the case of $i = 1$, we have $\Delta t_{i-1} = \Delta t_0 = 0$, $\delta c_{i-1} = \delta c_0 = h(\mathbf{x}, 0)$, and $\delta\lambda_{i-1} = \delta\lambda_0 = \mu(\mathbf{x}, 0)$. However, since the initial concentration at the well is a known value, the initial variation of the concentration at the well, $h(\mathbf{x}, 0)$, must be zero. Thus, the last line in (64) for $i = 1$ becomes

$$\int_\Omega c(\mathbf{x},0)\mu(\mathbf{x},0)d\mathbf{x}. \tag{65}$$

Similarly, when $i = n$, $\Delta t_i = \Delta t_n = 0$, $\delta c_i = \delta c_n = h(\mathbf{x}, t_f)$, and $\delta\lambda_i = \delta\lambda_n = \mu(\mathbf{x}, t_f)$, and the second to the last line reduces to

$$\int_{\Gamma_1} f_{c_t}\Big|_{t=t_f} h(\mathbf{x},t_f)ds_1 - \int_\Omega c(\mathbf{x},t_f)\mu(\mathbf{x},t_f)d\mathbf{x} - \int_\Omega \lambda(\mathbf{x},t_f)h(\mathbf{x},t_f)d\mathbf{x}. \tag{66}$$

Recall, from equation (41) that the first variation of the Lagrangian is just the sum of the first variations on each of the n intervals. Thus by using (41), we can build the Lagrangian by summing the terms in (64) for all i, using (65) and (66) for $i = 1$ and $i = n$, respectively. With this summing process, we see that the first two terms (h and μ terms) of (64) become

$$\int_0^{t_f}\left\{\int_{\Gamma_1}(f_c-\frac{\partial}{\partial t}f_{c_t})h(s,t)ds_1 + \int_\Omega h(\mathbf{x},t)\left(L^*\lambda+\lambda_t+Ae^{\alpha t}\int_t^{t_f}\lambda(\mathbf{x},\tau)e^{-\alpha\tau}d\tau\right)d\mathbf{x} - \int_{\Gamma_2}h(s,t)\underline{\underline{D}}_h\cdot\nabla\lambda\cdot\hat{\mathbf{n}}_2 ds_2+\int_{\Gamma_1}\left[h(s,t)(\underline{\underline{D}}_h\cdot\nabla\lambda+\lambda\mathbf{v})\right]\cdot\hat{\mathbf{n}}_1 ds_1\right\}dt \tag{67}$$

and

$$\int_0^{t_f}\int_\Omega\left(\mu_t c+\mu[Lc+a_0]+Ace^{\alpha t}\left\{\int_t^{t_f}\mu(\mathbf{x},\tau)e^{-\alpha\tau}d\tau+\lambda^{(i)}e^{-\alpha t}\Big|_{t=t_i}\Delta t_i+\cdots \cdots -\lambda^{(n)}e^{-\alpha t}\Big|_{t=t_{n-1}}\Delta t_{n-1}\right\}\right)d\mathbf{x}dt. \tag{68}$$

Assuming the Lagrange multiplier, $\lambda(\mathbf{x},t)$, is continuous at t_i for all i = 1, 2, ... n-1 (the validity of this assumption will be presented in the next section), expression (68) can be written as

$$\int_0^{t_f}\int_\Omega \mu\left(Lc+a_0-c_t+Ae^{-\alpha t}\int_0^t c(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right)d\mathbf{x}dt+\int_\Omega\left[c(\mathbf{x},t_f)\mu(\mathbf{x},t_f)-c(\mathbf{x},0)\mu(\mathbf{x},0)\right]d\mathbf{x}, \tag{69}$$

where the order of integration on $d\tau dt$ was reversed and integration by parts was used on the term involving the product $\mu_t c$.

The remaining terms in (64) contain information occurring at the switching times, t_i. If we examine a particular t_i, we see that the time to switch the status of the pump depends on information from the current interval, as well as information from the next interval. Recalling the terms in (65) and (66), which deal with the endpoints of the time interval, the remaining terms in (64) can be rewritten as

$$
\begin{aligned}
&\int_{\Gamma_1}\left\{(f - f_{c_t}c_t) + \left[c(\underline{\underline{D}}_h \cdot \nabla\lambda + \lambda\mathbf{v})\right]\cdot\hat{\mathbf{n}}_1\right\}\Big|_{t_i+0}^{t_i-0} ds_1\Delta t_i \\
&\quad + \int_\Omega \left\{c\left(L^*\lambda + \lambda_t + Ae^{\alpha t}\int_t^{t_f}\lambda(\mathbf{x},\tau)e^{-\alpha\tau}d\tau\right) + \lambda a_0\right\}\Big|_{t_i+0}^{t_i-0} d\mathbf{x}\Delta t_i \\
&\quad - \int_{\Gamma_2} c\underline{\underline{D}}_h \cdot \nabla\lambda\cdot\hat{\mathbf{n}}_2\Big|_{t_i+0}^{t_i-0} ds_2\Delta t_i \\
&\quad + \int_{\Gamma_1} f_{c_t}\Big|_{t_i+0}^{t_i-0}\delta c_i ds_1 - \int_\Omega\left\{c\Big|_{t_i+0}^{t_i-0}\delta\lambda_i + \lambda\Big|_{t_i+0}^{t_i-0}\delta c_i\right\}d\mathbf{x}
\end{aligned} \tag{70}
$$

for every i = 1, 2, ... n - 1, where (65) addresses the case when i = 0 and (66) addresses the case when i = n. In (70), the notation $F\Big|_{t_i+0}^{t_i-0}$ is defined as $F\Big|_{t_i+0}^{t_i-0} = \lim_{t\to t_i^-}F(t) - \lim_{t\to t_i^+}F(t)$ which is the jump in F at the time t_i.

Finally, combining the expressions in (65), (66), (67), (69), and (70) into equation (41), which represents the variation of the Lagrangian, we find

$$
\begin{aligned}
&\delta\mathcal{L}[Q,c,\lambda;\Delta t_i,h,\mu] = \\
&\int_0^{t_f}\left\{\int_{\Gamma_1}(f_c - \frac{\partial}{\partial t}f_{c_t})h(s,t)ds_1\right. \\
&\quad + \int_\Omega h(\mathbf{x},t)\left(L^*\lambda + \lambda_t + Ac^{\alpha t}\int_t^{t_f}\lambda(\mathbf{x},\tau)e^{-\alpha\tau}d\tau\right)d\mathbf{x} \\
&\quad \left. - \int_{\Gamma_2} h(s,t)\underline{\underline{D}}_h\cdot\nabla\lambda\cdot\hat{\mathbf{n}}_2 ds_2 + \int_{\Gamma_1}\left[h(s,t)(\underline{\underline{D}}_h\cdot\nabla\lambda + \lambda\mathbf{v})\right]\cdot\hat{\mathbf{n}}_1 ds_1\right\}dt \\
&\quad + \int_{\Gamma_1} f_{c_t}\Big|_{t=t_f} h(\mathbf{x},t_f)ds_1 - \int_\Omega\lambda(\mathbf{x},t_f)h(\mathbf{x},t_f)d\mathbf{x} \\
&\quad + \int_0^{t_f}\int_\Omega\mu\left(Lc + a_0 - c_t + Ae^{-\alpha t}\int_0^t c(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right)d\mathbf{x}dt \\
&\quad + \sum_{i=1}^{n-1}\left(\begin{aligned}
&\int_{\Gamma_1}\left\{(f - f_{c_t}c_t) + \left[c(\underline{\underline{D}}_h \cdot \nabla\lambda + \lambda\mathbf{v})\right]\cdot\hat{\mathbf{n}}_1\right\}\Big|_{t_i+0}^{t_i-0} ds_1\Delta t_i \\
&\quad + \int_\Omega \left\{c\left(L^*\lambda + \lambda_t + Ae^{\alpha t}\int_t^{t_f}\lambda(\mathbf{x},\tau)e^{-\alpha\tau}d\tau\right) + \lambda a_0\right\}\Big|_{t_i+0}^{t_i-0} d\mathbf{x}\Delta t_i \\
&\quad - \int_{\Gamma_2} c\underline{\underline{D}}_h \cdot \nabla\lambda\cdot\hat{\mathbf{n}}_2\Big|_{t_i+0}^{t_i-0} ds_2\Delta t_i \\
&\quad + \int_{\Gamma_1} f_{c_t}\Big|_{t_i+0}^{t_i-0}\delta c_i ds_1 - \int_\Omega\left\{c\Big|_{t_i+0}^{t_i-0}\delta\lambda_i + \lambda\Big|_{t_i+0}^{t_i-0}\delta c_i\right\}d\mathbf{x}
\end{aligned}\right).
\end{aligned} \tag{71}
$$

Equation (71) is the form of the first variation of the Lagrangian that was used to derive necessary optimality conditions for an optimal solution. Notice in (71) that the first variation of the Lagrangian has been expressed as a sum of the first variations of the Lagrangian with respect to the variables c, λ, and Δt_i, independently. That is, the terms which include $h(\mathbf{x},t)$ and δc_i represent the first variation with respect to the concentration alone; the terms which include $\mu(\mathbf{x},t)$ and $\delta\lambda_i$ represent the first variation with respect to the Lagrange multiplier alone; and the terms which include Δt_i represent the first variation with respect to the pump switching time alone. Thus, if we had applied Definition 1 to each variable (c, λ, and t_i) separately while holding the others fixed, we would have arrived at the identical expressions that are found in (71).

The next section of this chapter presents a theorem that establishes NOCs for the first variation of the Lagrangian. In the proof of this theorem, a thorough investigation of the admissible variations of h, λ, Δt_i, δc_i, and $\delta\lambda_i$, leads to a set of NOCs which must be satisfied by an optimal solution for the optimization problem described in Chapter III. The conditions presented in the theorem are surprisingly simple, when compared with the lengthy expression presented in this section.

4.2 *Admissible Variations*

The preceding section fully developed the first variation of the Lagrangian of the optimization problem stated in Chapter III. The present section analyzes the first variation, applying the theory stated in the previous chapter to arrive at NOCs for the existence of an optimal pulsed pumping schedule. In this section, we will state these

NOCs in the form of a theorem which must be satisfied by any optimal solution to the optimization problem. In proving this theorem, we investigate equation (71) and arrive at the NOCs by examining the sets of admissible variations of c, λ, and t_i (i.e., admissible h, μ, and Δt_i). Before proceeding with this investigation, three preliminary lemmas are presented which aid in the discussion.

Lemma 1. If $\alpha(x)$ is continuous in [a, b], and if

$$\int_a^b \alpha(x)h(x)dx = 0$$

for every function $h \in C(a, b)$ such that $h(a) = h(b) = 0$, then $\alpha(x) = 0$ for all $x \in [a, b]$ (Gelfand & Fomin, 1963:9).

The next lemma extends Lemma 1 to functionals of several variables.

Lemma 2. Suppose Ω is a compact region in the xy-plane. If $V = \Omega \times [a, b]$ is a closed volume such that $\alpha(\mathbf{x},t)$ is a fixed function which is continuous in V, where **x** is the point (x,y), and if

$$\int_a^b \int_\Omega \alpha(\mathbf{x},t)h(\mathbf{x},t)d\mathbf{x}dt = 0$$

for every continuous function $h(\mathbf{x},t)$ in V which equals zero on the boundary Γ of V, then $\alpha(\mathbf{x},t) = 0$ everywhere in V.

Proof. This proof follows the logic from the proof of Lemma 1, presented by Gelfand & Fomin (1963). Suppose the function α is nonzero, say positive, at some point (x_0, y_0, t_0) in V. Since α is continuous in V, then the function is also positive in some sphere

$$(x - x_0)^2 + (y - y_0)^2 + (t - t_0)^2 \le \varepsilon^2$$

contained in V for sufficiently small $\varepsilon > 0$. If we set $h(\mathbf{x},t) = 0$ outside the sphere and

$$h(\mathbf{x},t) = [\varepsilon^2 - (x - x_0)^2 - (y - y_0)^2 - (t - t_0)^2]^3$$

inside the sphere, then $h(\mathbf{x},t)$ satisfies the condition of the lemma. However, the integration in the lemma reduces to an integration over the sphere defined above and is obviously positive. This contradiction proves the lemma. □

Lemma 3. Suppose Γ is a simple closed curve in the xy-plane. If $S = \Gamma \times [a, b]$ is a cylindrical surface such that $\alpha(x,t)$ is a fixed function which is continuous in S, and if

$$\int_a^b \int_\Gamma \alpha(x,t) h(x,t) dx dt = 0$$

for every function $h(x,t)$ which is continuous on S such that $h(x,a) = h(x,b) = 0$ for any point $x \in \Gamma$, then $\alpha(x,t) = 0$ everywhere on S.

The proof of Lemma 3 is similar to that of Lemma 2 and is omitted.

In the previous section, the final form of the first variation of the Lagrangian was derived with these lemmas in mind. Notice, the two time integrals in equation (71) take the forms of the integrals in Lemmas 2 and 3 above. Applying Theorem 1 to the first variation of the Lagrangian implies that equation (71) must vanish for all possibilities of admissible variations on h, μ, and Δt_i. Applying these lemmas to several special cases produces necessary conditions for an optimal solution.

For example, it is possible that the variations on the switching times and the variation on the Lagrange multiplier might be zero. For this special case, the first variation reduces to a time integral over terms that include a product of the variation of the concentration with another function of time and space, integrated separately in space

over both the boundary and the domain of the confined aquifer. If we further assume that the variation of the concentration could vanish on the boundary $\Gamma = \Gamma_1 \cup \Gamma_2$ (which is certainly possible for admissible variations, h) and at the time endpoints of a particular interval, then equation (71) reduces to the form of the integral in Lemma 2. *Thus, for the first variation to vanish for this special case, Lemma 2 implies a necessary condition that the term $\alpha(x, t)$ must vanish **for all** (x, t) contained in the region of integration.*

With this necessary condition applied to (71), the first variation is reduced, and the search for different possibilities for the variation of the concentration continues. Repeating this process, we conclude with necessary conditions that must be met for all points in the domain and on the boundary of the aquifer, guaranteeing the first variation of the Lagrangian will vanish for all admissible variations, h. This technique motivates the proof of the following theorem.

Theorem 6. (Necessary Optimality Conditions of the First Variation) Let J[Q,c] be the functional given by equation (24), constrained by the boundary value problem defined by equations (25) through (27), and assume that f has continuous first partial derivatives for all of its arguments on the i^{th} interval of $[0, t_f]$, given as $[t_{i-1}, t_i]$ for all i = 1, 2, ... n. Let $c(\mathbf{x},t)$ and $\lambda(\mathbf{x},t)$ be given as $c(\mathbf{x},t) = c^{(i)}(\mathbf{x},t)$ and $\lambda(\mathbf{x},t) = \lambda^{(i)}(\mathbf{x},t)$, and let $Q(t) = Q^{(i)}(t)$, (defined by equation (43)) for $t \in [t_{i-1}, t_i]$ and for all i = 1, 2, ... n. If the functions $(\hat{Q}, \hat{c}, \hat{\lambda})$ produce an extremal for the functional in (24) constrained by (25) through (27), then the optimal pulsed pumping schedule is determined by

$$[\hat{f} - \hat{f}_{c_t}\hat{c}_t - \hat{c}(\hat{f}_c - \frac{\partial}{\partial t}\hat{f}_{c_t})]\Big|_{x=x_w}\Big|_{t_i+0}^{t_i-0} = 0 \qquad \forall i = 1, 2, \ldots n-1,$$

where $\hat{f}_c$ and $\hat{f}_{c_t}$ denote that the quantities are evaluated at optimal $\hat{c}$ and $\hat{Q}$, the jump notation is defined as before: $F\Big|_{t_i+0}^{t_i-0} = \lim_{t\to t_i^-} F(t) - \lim_{t\to t_i^+} F(t)$, $\mathbf{x} = \mathbf{x}_w$ means evaluation at the extraction well, and optimal $\hat{c}$ must satisfy

$$L\hat{c} + a_0 - \hat{c}_t + Ae^{-\alpha t}\int_0^t \hat{c}(\mathbf{x},\tau)e^{\alpha\tau}d\tau = 0$$

for all $(\mathbf{x},t) \in \Omega \times [t_{i-1}, t_i]$, and for all i = 1, 2, ... n, where $\hat{c}\Big|_{t_i+0}^{t_i-0} = 0$ for each i = 1, 2, ... n-1. Further, the Lagrange multiplier must be a solution of the adjoint boundary value problem, which satisfies the integro-differential equation

$$L^*\hat{\lambda} + \hat{\lambda}_t + Ae^{\alpha t}\int_t^{t_f} \hat{\lambda}(\mathbf{x},\tau)e^{-\alpha\tau}d\tau = 0$$

for all $(\mathbf{x},t) \in \Omega \times [t_{i-1}, t_i]$, with boundary conditions

$$(\hat{f}_c - \frac{\partial}{\partial t}\hat{f}_{c_t}) + (\underline{\underline{D}}_h \cdot \nabla\hat{\lambda} + \hat{\lambda}\mathbf{v}) \cdot \hat{\mathbf{n}}_1 = 0 \qquad \text{for all } (\mathbf{x},t) \in \Gamma_1 \times [t_{i-1}, t_i]$$

$$\underline{\underline{D}}_h \cdot \nabla\hat{\lambda} \cdot \hat{\mathbf{n}}_2 = 0 \qquad \text{for all } (\mathbf{x},t) \in \Gamma_2 \times [t_{i-1}, t_i],$$

terminal conditions

$$\hat{f}_{c_t}\Big|_{t=t_f} = 0 \qquad \text{for all } \mathbf{x} \in \Gamma_1$$

$$\hat{\lambda}(\mathbf{x}, t_f) = 0 \qquad \text{for all } \mathbf{x} \in \Omega,$$

and corner conditions

$$\hat{f}_{c_t}\Big|_{t_i+0}^{t_i-0} = 0 \qquad \text{for all } \mathbf{x} \in \Gamma_1 \text{ and for all } i = 1, 2, \ldots n-1$$

$$\hat{\lambda}\Big|_{t_i+0}^{t_i-0} = 0 \qquad \text{for all } \mathbf{x} \in \Omega \text{ and for all } i = 1, 2, \ldots n-1.$$

Proof. The proof of this theorem examines three special cases on a single time interval (t_{i-1},t_i). Each of these special cases leads to necessary conditions for all points in the domain and on the boundary of the aquifer, continually reducing equation (71) until we find a set of n-1 conditions for the switching time to produce an optimal solution. These times represent the optimal pulsed pumping schedule and can be determined from the concentration information provided at the pumping well.

Case 1. In order to look at the case where the concentration varies alone, suppose the variation of the Lagrange multiplier is zero and the switching times are fixed. That is, let

$$\begin{aligned} &\mu(\mathbf{x},t) = 0 && \forall \mathbf{x} \in \Omega, \quad 0 \le t \le t_f \\ \text{and} \qquad & && \qquad\qquad (72) \\ &\Delta t_i = 0 && \forall i = 1, 2, \ldots n-1. \end{aligned}$$

Further, suppose the functions $(\hat{Q},\hat{c},\hat{\lambda})$ optimize the Lagrangian, $\mathcal{L}$. Then according to Theorem 1, the first variation of the Lagrangian must vanish for all admissible variations of the concentration. Thus, $\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};0,h,0] = 0$ for all $h \in H$, the set of admissible variations. These assumptions reduce the first variation to

$$
\begin{aligned}
&\delta\mathscr{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i=0,h,\mu=0]\\
&=\int_0^{t_f}\left\{\int_{\Gamma_1}(\hat{f}_c-\frac{\partial}{\partial t}\hat{f}_{c_t})h(s,t)ds_1\right.\\
&\qquad+\int_{\Omega}h(\mathbf{x},t)\left(L^*\hat{\lambda}+\hat{\lambda}_t+Ae^{\alpha t}\int_t^{t_f}\hat{\lambda}(\mathbf{x},\tau)e^{-\alpha\tau}d\tau\right)d\mathbf{x}\\
&\qquad\left.-\int_{\Gamma_2}h(s,t)\underline{\underline{D}}_h\cdot\nabla\hat{\lambda}\cdot\hat{\mathbf{n}}_2ds_2+\int_{\Gamma_1}\left[h(s,t)(\underline{\underline{D}}_h\cdot\nabla\hat{\lambda}+\hat{\lambda}\mathbf{v})\right]\cdot\hat{\mathbf{n}}_1ds_1\right\}dt\\
&+\int_{\Gamma_1}\hat{f}_{c_t}\Big|_{t=t_f}h(\mathbf{x},t_f)ds_1-\int_{\Omega}\hat{\lambda}(\mathbf{x},t_f)h(\mathbf{x},t_f)d\mathbf{x}\\
&+\sum_{i=1}^{n-1}\left(\int_{\Gamma_1}\hat{f}_{c_t}\Big|_{t_i+0}^{t_i-0}h(\mathbf{x},t_i)ds_1-\int_{\Omega}\hat{\lambda}\Big|_{t_i+0}^{t_i-0}h(\mathbf{x},t_i)d\mathbf{x}\right),
\end{aligned}
\tag{73}
$$

where (58) implies that $\delta c_i = h(\mathbf{x},t_i)$ when $\Delta t_i = 0$ and $\hat{f}_c$ and $\hat{f}_{c_t}$ denote that the quantities are evaluated at optimal $\hat{c}$ and $\hat{Q}$. Equation (73) represents the first variation of the Lagrangian with respect to the concentration alone. This is the same expression that would have been derived if we had started with the Lagrangian in (39), and had allowed only the concentration to vary.

Next, three subcases of this first case were examined to investigate all possibilities for $h \in H$. Again, these special cases led to necessary conditions *for all* points within the aquifer. The first assumption is that admissible h is nonzero on a single sub-interval of $[0, t_f]$, that is, suppose h is nonzero on the i^{th} interval only, but zero elsewhere. Then, $h \neq 0$ for all $t \in (t_{i-1}, t_i)$ and any $\mathbf{x} \in \Omega$. To establish necessary conditions for the first variation, we must satisfy $\delta\mathscr{L} = 0$ for the case defined above on every interval of $[0, t_f]$.

(a) Initially, choose $h \in H$ such that

(i) $h(\mathbf{x}, t) = 0 \quad \forall\, \mathbf{x} \in \Omega \cup \Gamma$ and $\forall\, t \notin (t_{i-1}, t_i)$

(ii) $h(\mathbf{x}, t) = 0 \quad \forall\, \mathbf{x} \in \Gamma = \Gamma_1 \cup \Gamma_2$ and $\forall\, t \in [t_{i-1}, t_i]$.

By applying (i) and (ii) above, we are limiting our search for admissible h such that h is zero everywhere on the boundary of the two-dimensional domain as well as the time boundary for case 1(a), i.e., the boundary of D x $[t_{i-1}, t_i]$ (Figure 6), where $D = \Omega \cup \Gamma$. Thus, equation (73) becomes (suppressing the (i) superscripts)

$$\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};0,h,0] = \int_{t_{i-1}}^{t_i}\int_{\Omega} h(\mathbf{x},t)\left(L^*\hat{\lambda}+\hat{\lambda}_t + Ae^{\alpha t}\int_t^{t_f}\hat{\lambda}(\mathbf{x},\tau)e^{-\alpha\tau}d\tau\right)dxdt. \tag{74}$$

The integral in equation (74) meets the hypothesis of Lemma 2 since h is zero everywhere on the boundary of the region of integration. Setting the integral in (74) to zero and applying the lemma yields the first NOC of the first variation as

$$L^*\hat{\lambda}+\hat{\lambda}_t + Ae^{\alpha t}\int_t^{t_f}\hat{\lambda}(\mathbf{x},\tau)e^{-\alpha\tau}d\tau = 0 \tag{75}$$

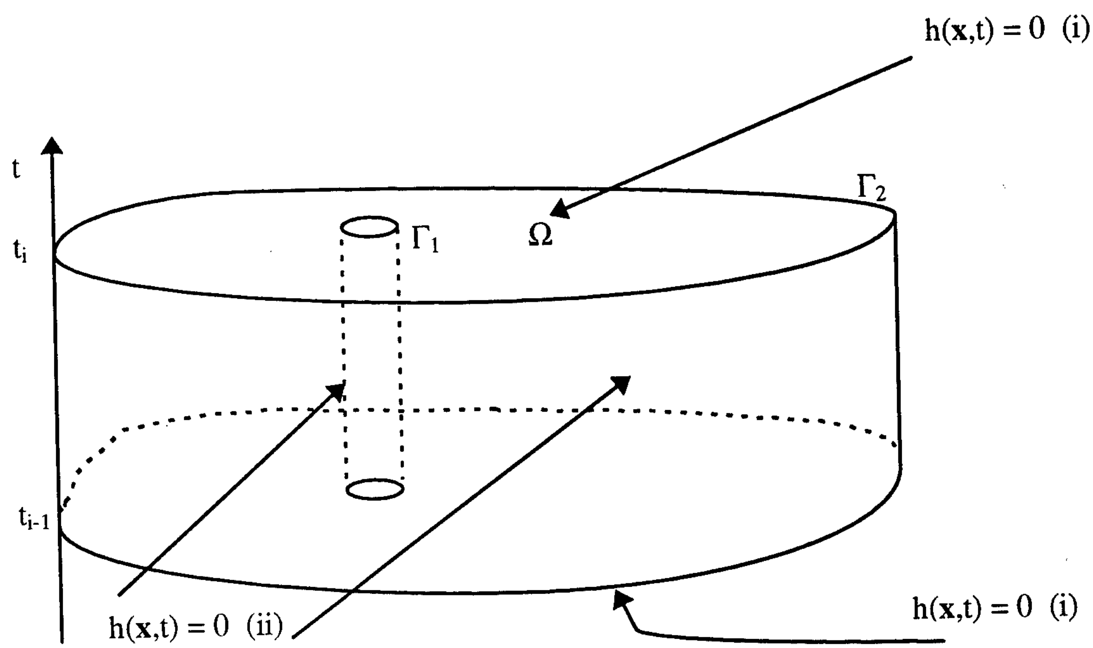

Figure 6. Case 1(a). The variation $h(\mathbf{x},t) = 0$ everywhere on the boundary of the domain D x $[t_{i-1}, t_i]$.

for all $(\mathbf{x},t) \in \Omega \times [t_{i-1}, t_i]$. Equation (75) is a necessary condition for optimality, and must be satisfied since $\hat{c}$ is optimal. Since i is arbitrary, (75) must hold for any i = 1, 2, ... n. Applying the necessary condition (75) on every interval reduces the first variation of the Lagrangian in (73) to

$$\begin{aligned}\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};0,h,0] = \int_0^{t_f}\Big\{&\int_{\Gamma_1}(\hat{f}_c - \frac{\partial}{\partial t}\hat{f}_{c_t})h(s,t)ds_1 - \int_{\Gamma_2} h(s,t)\underline{\underline{D}}_h \cdot \nabla\hat{\lambda}\cdot\hat{\mathbf{n}}_2 ds_2 \\ &+ \int_{\Gamma_1}\Big[h(s,t)(\underline{\underline{D}}_h \cdot \nabla\hat{\lambda} + \hat{\lambda}\mathbf{v})\Big]\cdot\hat{\mathbf{n}}_1 ds_1\Big\}dt \\ &+ \int_{\Gamma_1}\hat{f}_{c_t}\Big|_{t=t_f} h(\mathbf{x},t_f)ds_1 - \int_\Omega \hat{\lambda}(\mathbf{x},t_f)h(\mathbf{x},t_f)d\mathbf{x} \\ &+ \sum_{i=1}^{n-1}\Big(\int_{\Gamma_1}\hat{f}_{c_t}\Big|_{t_i+0}^{t_i-0} h(\mathbf{x},t_i)ds_1 - \int_\Omega \hat{\lambda}\Big|_{t_i+0}^{t_i-0} h(\mathbf{x},t_i)d\mathbf{x}\Big).\end{aligned} \qquad (76)$$

(b) Next, choose $h \in H$ such that

(i) $h(\mathbf{x}, t) = 0 \quad \forall\, \mathbf{x} \in \Omega \cup \Gamma$ and $\forall\, t \notin (t_{i-1}, t_i)$

(iii) $h(\mathbf{x}, t) = 0 \quad \forall\, \mathbf{x} \in \Gamma_2$ and $\forall\, t \in [t_{i-1}, t_i]$.

With these assumptions, the admissible variations are allowed to be zero on the boundary of the aquifer, but nonzero at the well (Figure 7), reducing the first variation in (76) to

$$\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};0,h,0] = \int_{t_{i-1}}^{t_i}\int_{\Gamma_1} h(s,t)\Big\{(\hat{f}_c - \frac{\partial}{\partial t}\hat{f}_{c_t}) + (\underline{\underline{D}}_h \cdot \nabla\hat{\lambda} + \hat{\lambda}\mathbf{v})\cdot\hat{\mathbf{n}}_1\Big\}ds_1 dt. \qquad (77)$$

Setting the integral in (77) to zero allows the application of Lemma 3, producing the second NOC for the first variation

$$(\hat{f}_c - \frac{\partial}{\partial t}\hat{f}_{c_t}) + (\underline{\underline{D}}_h \cdot \nabla\hat{\lambda} + \hat{\lambda}\mathbf{v})\cdot\hat{\mathbf{n}}_1 = 0 \qquad (78)$$

for all $(\mathbf{x},t) \in \Gamma_1 \times [t_{i-1}, t_i]$. Again, i is arbitrary and (78) must hold for any i = 1, 2, ... n.

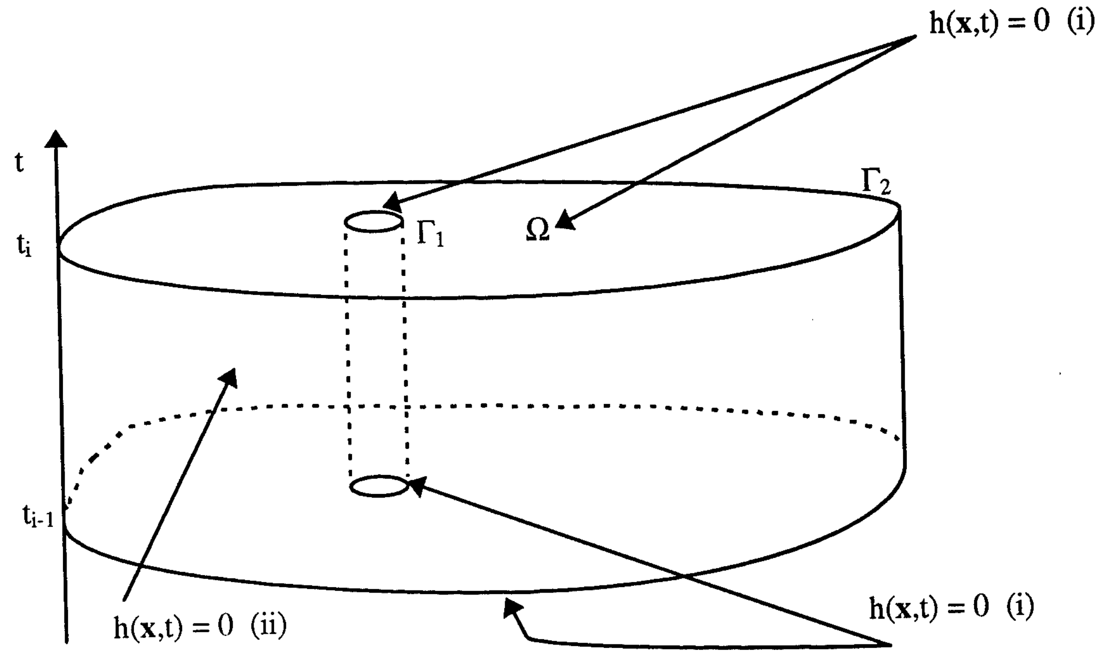

Figure 7. Case 1(b). The variation $h(\mathbf{x},t) = 0$ everywhere on the boundary of the domain D x $[t_{i-1}, t_i]$ except at the well for $t \in (t_{i-1}, t_i)$.

Since equation (78) is a necessary condition for optimality, we apply this condition on every interval of the first variation of the Lagrangian in (76), which yields

$$\begin{aligned}\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};0,h,0] = &-\int_0^{t_f}\int_{\Gamma_2} h(s,t)\underline{\underline{D}}_h \cdot \nabla\hat{\lambda}\cdot\hat{\mathbf{n}}_2 ds_2 dt \\ &+\int_{\Gamma_1}\hat{f}_{c_t}\Big|_{t=t_f} h(\mathbf{x},t_f)ds_1 - \int_\Omega \hat{\lambda}(\mathbf{x},t_f)h(\mathbf{x},t_f)d\mathbf{x} \\ &+\sum_{i=1}^{n-1}\left(\int_{\Gamma_1}\hat{f}_{c_t}\Big|_{t_i+0}^{t_i-0} h(\mathbf{x},t_i)ds_1 - \int_\Omega \hat{\lambda}\Big|_{t_i+0}^{t_i-0} h(\mathbf{x},t_i)d\mathbf{x}\right).\end{aligned} \tag{79}$$

(c) Finally, choose $h \in H$ such that

(i) $h(\mathbf{x}, t) = 0 \quad \forall\, \mathbf{x} \in \Omega \cup \Gamma$ and $\forall\, t \notin (t_{i-1}, t_i)$.

With this assumption, the admissible variations are allowed to be zero on the time boundary of the interval $[t_{i-1}, t_i]$, but nonzero at all other times within the aquifer. Thus, for this case, the aquifer depicted in Figure 8 would have $h(\mathbf{x},t) = 0$ everywhere on the top

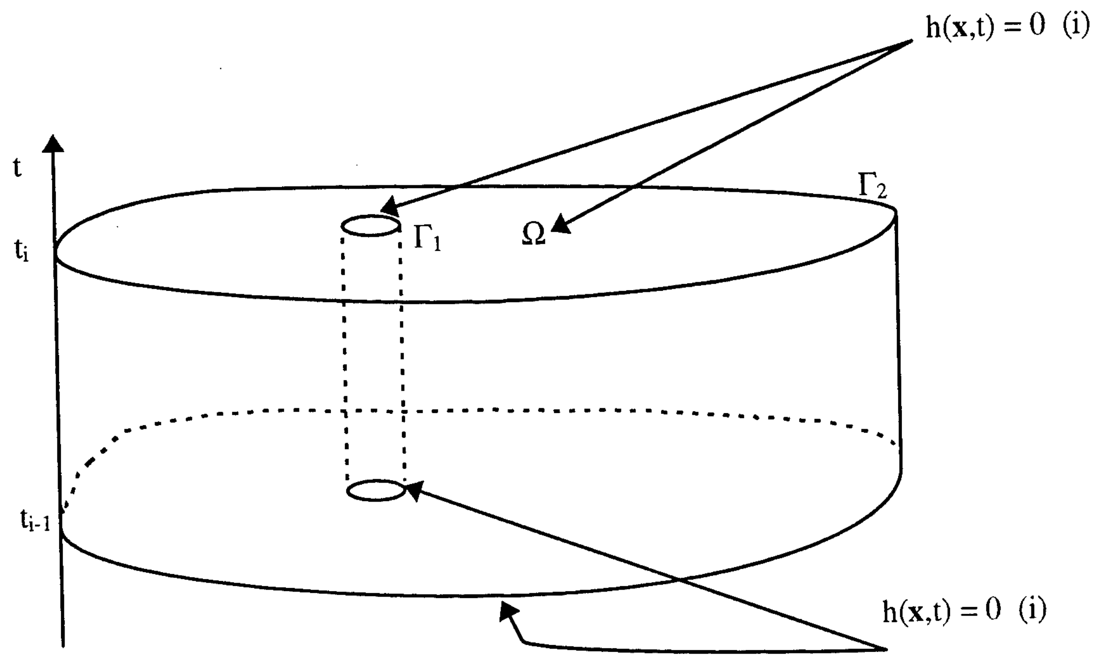

Figure 8. Case 1(c). The variation $h(\mathbf{x},t) = 0$ everywhere on the time boundary of the domain D x $[t_{i-1}, t_i]$.

and bottom of the figure. This assumption reduces the first variation in (79) to

$$\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};0,h,0] = -\int_{t_{i-1}}^{t_i}\int_{\Gamma_2} h(s,t)\underline{\underline{D}}_h \cdot \nabla\hat{\lambda}\cdot\hat{\mathbf{n}}_2 ds_2 dt. \tag{80}$$

Setting the integral in (80) to zero allows the application of Lemma 3, producing the next NOC for the first variation

$$\underline{\underline{D}}_h \cdot \nabla\hat{\lambda}\cdot\hat{\mathbf{n}}_2 = 0 \tag{81}$$

for all $(\mathbf{x},t) \in \Gamma_2$ x $[t_{i-1}, t_i]$. Since equation (81) is a necessary condition for optimality, we apply this condition to the first variation in (79), reducing the first variation of the Lagrangian to

$$\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};0,h,0] = \int_{\Gamma_1} \hat{f}_{c_t}\Big|_{t=t_f} h(\mathbf{x},t_f)ds_1 - \int_{\Omega}\hat{\lambda}(\mathbf{x},t_f)h(\mathbf{x},t_f)d\mathbf{x}$$
$$+\sum_{i=1}^{n-1}\left(\int_{\Gamma_1}\hat{f}_{c_t}\Big|_{t_i+0}^{t_i-0} h(\mathbf{x},t_i)ds_1 - \int_{\Omega}\hat{\lambda}\Big|_{t_i+0}^{t_i-0} h(\mathbf{x},t_i)d\mathbf{x}\right). \tag{82}$$

Each term in equation (82) involves evaluation of the variation, h, at a specific point in time, t_i. As such, the terms are independent and since $h(\mathbf{x},t_i)$ are arbitrary variations for each i = 1, 2, ...n, then each term in (82) must equal zero independently, leading to the 'corner' conditions

$$\hat{f}_{c_t}\Big|_{t_i+0}^{t_i-0} = 0 \qquad \forall\mathbf{x}\in\Gamma_1 \text{ and } \forall i = 1, 2, \dots n-1 \tag{83a}$$

and

$$\hat{\lambda}\Big|_{t_i+0}^{t_i-0} = 0 \qquad \forall\mathbf{x}\in\Omega \text{ and } \forall i = 1, 2, \dots n-1, \tag{83b}$$

and the terminal conditions

$$\hat{f}_{c_t}\Big|_{t=t_f} = 0 \qquad \forall\mathbf{x}\in\Gamma_1 \tag{84a}$$

and

$$\hat{\lambda}(\mathbf{x},t_f) = 0 \qquad \forall\mathbf{x}\in\Omega. \tag{84b}$$

The corner conditions in (83) assert the continuity condition for the Lagrange multiplier at each time, t_i, as well as the continuity of the first partial of f with respect to the time rate of change of the concentration at t_i. The continuity of λ justifies the simplification made in equation (69), and also serves to further simplify the first variation of the Lagrangian.

The necessary conditions contained in equations (75), (78), (81), (83), and (84) are effectively the NOCs for optimal $\hat{c}$. Returning to equation (71), we see the first variation of the Lagrangian (given that the functions $(\hat{Q},\hat{c},\hat{\lambda})$ are optimal) can now be written as

$$\begin{aligned}&\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i,h,\mu]=\\&\int_0^{t_f}\int_\Omega \mu\left(L\hat{c}+a_0-\hat{c}_t+Ae^{-\alpha t}\int_0^t \hat{c}(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right)d\mathbf{x}dt-\sum_{i=1}^{n-1}\int_\Omega \hat{c}\Big|_{t_i+0}^{t_i-0}\delta\lambda_i d\mathbf{x}\\&+\sum_{i=1}^{n-1}\int_{\Gamma_1}\left\{(\hat{f}-\hat{f}_{c_t}\hat{c}_t)-\hat{c}(\hat{f}_c-\frac{\partial}{\partial t}\hat{f}_{c_t})\right\}\Big|_{t_i+0}^{t_i-0}ds_1\Delta t_i,\end{aligned}\tag{85}$$

where equations (75), (78), (81), and (83) were introduced into the Δt_i terms to simplify the expression. Next, we seek the admissible values of the variation of the Lagrange multiplier, μ, leading to the second case presented below.

__Case 2__. Now, suppose the functions $(\hat{Q},\hat{c},\hat{\lambda})$ optimize the Lagrangian and the switching times are fixed. That is, let

$$\Delta t_i = 0 \qquad \forall i = 1, 2, \ldots n-1,\tag{86}$$

then $\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};0,h,\mu]=0$ for each $\mu\in M$, the set of admissible variations of λ. These assumptions reduce (85) to

$$\begin{aligned}&\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i=0,h,\mu]=\\&\int_0^{t_f}\int_\Omega \mu\left(L\hat{c}+a_0-\hat{c}_t+Ae^{-\alpha t}\int_0^t \hat{c}(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right)d\mathbf{x}dt-\sum_{i=1}^{n-1}\int_\Omega \hat{c}\Big|_{t_i+0}^{t_i-0}\mu(\mathbf{x},t_i)d\mathbf{x},\end{aligned}\tag{87}$$

where (58) implies that $\delta\lambda_i = \mu(\mathbf{x},t_i)$ when $\Delta t_i = 0$. Now, suppose that admissible μ is nonzero only on the i^{th} interval, and zero elsewhere. Necessary conditions for the first variation follow from the application of Theorem 1. Since the functions $(\hat{Q},\hat{c},\hat{\lambda})$ optimize $\mathcal{L}$, then we must satisfy $\delta\mathcal{L} = 0$ for the case defined above on every interval of $[0, t_f]$. Thus, choose $\mu(\mathbf{x}, t)$ such that

(i) $\mu(\mathbf{x}, t) = 0 \quad \forall\, \mathbf{x} \in \Omega$ and $\forall\, t \notin (t_{i-1}, t_i)$

(ii) $\mu(\mathbf{x}, t) = 0 \quad \forall\, \mathbf{x} \in \Gamma = \Gamma_1 \cup \Gamma_2$ and $\forall\, t \in [t_{i-1}, t_i]$.

Applying (i) and (ii), equation (87) becomes

$$\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};0,h,\mu] = \int_{t_{i-1}}^{t_i}\int_{\Omega}\mu\left(L\hat{c} + a_0 - \hat{c}_t + Ae^{-\alpha t}\int_0^t \hat{c}(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right)d\mathbf{x}dt. \tag{88}$$

The integral of (88) satisfies the hypothesis of Lemma 2 since μ is zero everywhere on the boundary of the region of integration. Setting (88) to zero and applying the lemma produces the NOC

$$L\hat{c} + a_0 - \hat{c}_t + Ae^{-\alpha t}\int_0^t \hat{c}(\mathbf{x},\tau)e^{\alpha\tau}d\tau = 0 \tag{89}$$

for all $(\mathbf{x},t) \in \Omega \times [t_{i-1}, t_i]$. The NOC of equation (89) simply states that optimal $\hat{c}$ must satisfy the contaminant transport equations, presented in Chapter III. Also, since i is arbitrary, (89) must hold for all i = 1, 2, ... n. Applying this NOC to the first variation of the Lagrangian, we are left with

$$\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};0,h,\mu] = -\sum_{i=1}^{n-1}\int_{\Omega}\hat{c}\Big|_{t_i+0}^{t_i-0}\mu(\mathbf{x},t_i)d\mathbf{x}. \tag{90}$$

Setting the term in (90) to zero leads to the necessary condition

$$\hat{c}\Big|_{t_i+0}^{t_i-0} = 0 \qquad \forall i = 1, 2, \ldots n-1, \tag{91}$$

which states the continuity of the concentration at the switching times, t_i. The necessary conditions for optimal $\hat{\lambda}$ are contained in equations (89) and (91). Applying these conditions and the necessary conditions for optimal $\hat{c}$ in equations (75), (78), (81), (83), and (84), to the first variation of the Lagrangian given by (71), reduces the expression to

$$\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i,h,\mu] = \sum_{i=1}^{n-1}\int_{\Gamma_1}\left\{(\hat{f}-\hat{f}_{c_t}\hat{c}_t)-\hat{c}(\hat{f}_c-\frac{\partial}{\partial t}\hat{f}_{c_t})\right\}\Big|_{t_i+0}^{t_i-0} ds_1 \Delta t_i\,. \tag{92}$$

With the NOCs found thus far, the first variation of the Lagrangian has been reduced significantly for the optimal functions $(\hat{Q},\hat{c},\hat{\lambda})$. The final step that remains is to allow nonzero values for the variation of the switching times, Δt_i. This step produces n-1 necessary conditions for an optimal pulsed pumping schedule that, when satisfied, will produce the n-1 optimal times to switch the state of the pumps from on to off or vice-versa and back again.

Case 3. Finally, suppose the functions $(\hat{Q},\hat{c},\hat{\lambda})$ optimize $\mathcal{L}$ and the switching times are allowed to vary. If $\hat{Q}$ produces an optimal pulsed pumping schedule determined by the times, t_i, then $\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i,h,\mu]=0$ is necessary by Theorem 1. Thus, (92) becomes

$$\delta\mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i,h,\mu] = \sum_{i=1}^{n-1}\int_{\Gamma_1}\left\{(\hat{f}-\hat{f}_{c_t}\hat{c}_t)-\hat{c}(\hat{f}_c-\frac{\partial}{\partial t}\hat{f}_{c_t})\right\}\Big|_{t_i+0}^{t_i-0} ds_1 \Delta t_i = 0, \tag{93}$$

and each term in (93) must go to zero independently, producing the n-1 corner conditions that must be satisfied by optimal $\hat{Q}$

$$\int_{\Gamma_1}\left\{(\hat{f}-\hat{f}_{c_t}\hat{c}_t)-\hat{c}(\hat{f}_c-\frac{\partial}{\partial t}\hat{f}_{c_t})\right\}\Big|_{t_i+0}^{t_i-0}ds_1=0 \qquad \forall i = 1, 2, \ldots n-1. \tag{94}$$

In the two-dimensional aquifer, the boundary of the well is small when compared to the overall geometry of the aquifer. As such, we allow the boundary Γ_1 to shrink to zero, resulting in the evaluation of equation (94) at the location point of the center of the well. Thus, the necessary conditions of (94) become

$$[\hat{f}-\hat{f}_{c_t}\hat{c}_t-\hat{c}(\hat{f}_c-\frac{\partial}{\partial t}\hat{f}_{c_t})]\Big|_{x=x_w}\Big|_{t_i+0}^{t_i-0}=0 \qquad \forall i = 1, 2, \ldots n-1, \tag{95}$$

and the theorem has been proved. $\square$

Notice, equation (95) can be rewritten with the argument lists included as

$$\begin{aligned}
&f\left(t_i,\hat{Q}^{(i)},\hat{c}^{(i)}(\mathbf{x}_w,t_i),\hat{c}_t^{(i)}(\mathbf{x}_w,t_i)\right)-f_{c_t}\left(t_i,\hat{Q}^{(i)},\hat{c}^{(i)}(\mathbf{x}_w,t_i),\hat{c}_t^{(i)}(\mathbf{x}_w,t_i)\right)\hat{c}_t^{(i)}(\mathbf{x}_w,t_i)\\
&-\left\{\begin{aligned}&f\left(t_i,\hat{Q}^{(i+1)},\hat{c}^{(i+1)}(\mathbf{x}_w,t_i),\hat{c}_t^{(i+1)}(\mathbf{x}_w,t_i)\right)\\&\qquad -f_{c_t}\left(t_i,\hat{Q}^{(i+1)},\hat{c}^{(i+1)}(\mathbf{x}_w,t_i),\hat{c}_t^{(i+1)}(\mathbf{x}_w,t_i)\right)\hat{c}_t^{(i+1)}(\mathbf{x}_w,t_i)\end{aligned}\right\}\\
&-\hat{c}^{(i)}(\mathbf{x}_w,t_i)\left\{\begin{aligned}&f_c\left(t_i,\hat{Q}^{(i)},\hat{c}^{(i)}(\mathbf{x}_w,t_i),\hat{c}_t^{(i)}(\mathbf{x}_w,t_i)\right)\\&\qquad -\frac{\partial}{\partial t}f_{c_t}\left(t_i,\hat{Q}^{(i)},\hat{c}^{(i)}(\mathbf{x}_w,t_i),\hat{c}_t^{(i)}(\mathbf{x}_w,t_i)\right)\end{aligned}\right\}\\
&+\hat{c}^{(i+1)}(\mathbf{x}_w,t_i)\left\{\begin{aligned}&f_c\left(t_i,\hat{Q}^{(i+1)},\hat{c}^{(i+1)}(\mathbf{x}_w,t_i),\hat{c}_t^{(i+1)}(\mathbf{x}_w,t_i)\right)\\&\qquad -\frac{\partial}{\partial t}f_{c_t}\left(t_i,\hat{Q}^{(i+1)},\hat{c}^{(i+1)}(\mathbf{x}_w,t_i),\hat{c}_t^{(i+1)}(\mathbf{x}_w,t_i)\right)\end{aligned}\right\}=0
\end{aligned} \tag{96}$$

for every i = 1, 2, ... n-1, where $\mathbf{x}_w$ is the location of the center of the well. Since the concentration must be continuous at t_i, we could simplify equation (96) as

$$
\begin{aligned}
&f\left(t_i,\hat{Q}^{(i)},\hat{c}(\mathbf{x}_w,t_i),\hat{c}_t^{(i)}(\mathbf{x}_w,t_i)\right)-f_{c_t}\left(t_i,\hat{Q}^{(i)},\hat{c}(\mathbf{x}_w,t_i),\hat{c}_t^{(i)}(\mathbf{x}_w,t_i)\right)\hat{c}_t^{(i)}(\mathbf{x}_w,t_i)\\
&-\left\{f\left(t_i,\hat{Q}^{(i+1)},\hat{c}(\mathbf{x}_w,t_i),\hat{c}_t^{(i+1)}(\mathbf{x}_w,t_i)\right)-f_{c_t}\left(t_i,\hat{Q}^{(i+1)},\hat{c}(\mathbf{x}_w,t_i),\hat{c}_t^{(i+1)}(\mathbf{x}_w,t_i)\right)\hat{c}_t^{(i+1)}(\mathbf{x}_w,t_i)\right\}\\
&-\hat{c}(\mathbf{x}_w,t_i)\left\{f_c\left(t_i,\hat{Q}^{(i)},\hat{c}(\mathbf{x}_w,t_i),\hat{c}_t^{(i)}(\mathbf{x}_w,t_i)\right)-\frac{\partial}{\partial t}f_{c_t}\left(t_i,\hat{Q}^{(i)},\hat{c}(\mathbf{x}_w,t_i),\hat{c}_t^{(i)}(\mathbf{x}_w,t_i)\right)\right\}\\
&+\hat{c}(\mathbf{x}_w,t_i)\left\{f_c\left(t_i,\hat{Q}^{(i+1)},\hat{c}(\mathbf{x}_w,t_i),\hat{c}_t^{(i+1)}(\mathbf{x}_w,t_i)\right)-\frac{\partial}{\partial t}f_{c_t}\left(t_i,\hat{Q}^{(i+1)},\hat{c}(\mathbf{x}_w,t_i),\hat{c}_t^{(i+1)}(\mathbf{x}_w,t_i)\right)\right\}=0
\end{aligned}
\tag{97}
$$

for all i = 1, 2, ... n-1.

Equation (97) provides the tool to find an optimal pulsed pumping schedule. At first glance, one might think (97) is a partial differential equation where $\hat{c}$ is the dependent variable. However, equation (89) is a necessary condition on $\hat{c}$ that states the optimal concentration must satisfy the contaminant transport equations stated in the optimization problem. Thus, all we need to know is the value of the concentration and its time derivatives at the pumping well for discrete time values and then to find the times where equation (97) goes to zero becomes an algebra problem for a particular integrand f. Any contaminant transport code that incorporates the assumptions of our problem can provide the concentration data. For the illustrations presented in Chapter VII, the SUTRA code which incorporates rate-limited sorption (Caspers, 1994) was used to find the concentration information. This information was then used to find the zeroes of equation (97). The zeroes of (97) are the t_i's that determine the optimal pulsed pumping schedule.

4.3 *Summary*

This chapter developed the first variation of the Lagrangian of the optimization problem presented in Chapter III. Additionally, the first variation of the Lagrangian was examined for all possibilities of admissible variations of the concentration, the Lagrange multiplier, and the switching times. This investigation proved a theorem, establishing the NOCs of the first variation which must be satisfied by any optimal solution ($\hat{Q}$, $\hat{c}$, $\hat{\lambda}$). These NOCs produced a set of n-1 equations whose solutions form a candidate set of switching times for an optimal pulsed pumping schedule. These candidate switching times must still be tested to determine if they yield a minimum for a given objective functional.

In order to test these candidate solutions, a sufficiency test needs to be applied. The next chapter develops the theory of the second variation, and presents a theorem that establishes necessary conditions derived from the second variation of the Lagrangian. These necessary conditions serve as a tool to determine if the candidate switching times produced by (97) reflect a maximum or a minimum for the objective functional in question. Chapter VI builds on the necessary conditions presented in the next chapter to develop sufficient conditions for a minimal solution.

V. Necessary Optimality Conditions of the Second Variation

The first variation of the Lagrangian, derived and analyzed in Chapter IV, provided a tool in the form of necessary conditions which must be met by any optimal pulsed pumping schedule. The equations in (97) represent this tool, and the zeroes of (97) provide a candidate pumping schedule for an optimal solution of the functional in (24), subject to the constraints of (25) - (27). Since the goal of this research is to minimize the functional in (24), we must determine necessary and sufficient conditions for the existence of a minimum for the candidate times determined from the first variation of the Lagrangian.

The second variation of the Lagrangian serves to verify that the candidate optimal schedule found from (97) yields a minimum for the functional in (24). This chapter develops the second variation of the Lagrangian (from Definition 3) and applies Theorem 3 to prove a necessary conditions theorem, which the second variation must satisfy to produce a minimum for the functional (24). Sufficient conditions were found by applying Theorem 4, and Chapter VI presents the analysis that established sufficiency for a minimum.

5.1 Second Variation of the Lagrangian

This section develops the second variation of the Lagrangian in two dimensions. Again, as in the case of the first variation, the analysis in three dimensions is similar and will not be presented. The Lagrangian in two dimensions is restated as

$$\mathcal{L}[Q,c,\lambda] = \int_0^{t_f}\int_{\Gamma_1} f(t,Q(t),c(s,t),c_t(s,t))ds_1dt$$
$$+\int_0^{t_f}\int_\Omega \lambda(\mathbf{x},t)\left\{[Lc](\mathbf{x},t)+a_0(\mathbf{x},t)-c_t(\mathbf{x},t)+Ae^{-\alpha t}\int_0^t c(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right\}d\mathbf{x}dt. \tag{98}$$

Recall, when deriving the first variation, the order of integration on $d\tau dt$ was reversed. The main purpose of this step was to write the first variation as a sum of first variations with respect to each of the variables c, λ, and t_i. That is, in equation (71), the h and δc_i terms represent the first variation of the Lagrangian with respect to concentration alone, the μ and $\delta\lambda_i$ terms represent the first variation of the Lagrangian with respect to the Lagrange multiplier, and the Δt_i terms represent the first variation of the Lagrangian with respect to the switching times. With each of these expressions isolated, the analysis that followed was more direct. In analyzing the second variation, we find that using the Lagrangian in the form of (98) provides the best approach.

As was the case for the first variation, the second variation of the Lagrangian in (98) is equal to the sum of the second variations of the Lagrangians defined on each of the intervals in Figure 3. That is,

$$\delta^2\mathcal{L}[Q,c,\lambda] = \sum_{i=1}^n \delta^2\mathcal{L}^{(i)}[Q^{(i)},c^{(i)},\lambda^{(i)}], \tag{99}$$

where

$$\mathcal{L}^{(i)}[Q^{(i)},c^{(i)},\lambda^{(i)}] = \int_{t_{i-1}}^{t_i}\int_{\Gamma_1} f(t,Q^{(i)}(t),c^{(i)}(s,t),c_t^{(i)}(s,t))ds_1dt$$
$$+\int_{t_{i-1}}^{t_i}\int_\Omega \lambda^{(i)}(\mathbf{x},t)\left\{\begin{matrix}[L^{(i)}c^{(i)}](\mathbf{x},t)+a_0(\mathbf{x},t)-c_t^{(i)}(\mathbf{x},t)\\ +Ae^{-\alpha t}\int_0^t c(\mathbf{x},\tau)e^{\alpha\tau}d\tau\end{matrix}\right\}d\mathbf{x}dt. \tag{100}$$

Again, recalling that the variation of the Lagrangian due to Q(t) depends on the switching times, we write the second variation as

$$
\begin{aligned}
\delta^2 \mathcal{L}^{(i)}[Q^{(i)}, c^{(i)}, \lambda^{(i)}] &= \delta^2 \mathcal{L}^{(i)}[t_{i-1}, t_i, c^{(i)}, \lambda^{(i)}; \Delta t_{i-1}, \Delta t_i, h^{(i)}, \mu^{(i)}] \\
&= \frac{1}{2} \lim_{a \to 0} \frac{\partial^2}{\partial a^2} \mathcal{L}^{(i)}[t_{i-1} + a\Delta t_{i-1}, t_i + a\Delta t_i, c^{(i)} + ah^{(i)}, \lambda^{(i)} + a\mu^{(i)}],
\end{aligned}
\tag{101}
$$

where Δt_{i-1} and Δt_i are the variations of the endpoints of the i^{th} interval, as before. Also, simplifying the presentation, we use the definition of the variations given in equations (49) again and have

$$
\delta^2 \mathcal{L}^{(i)}[Q^{(i)}, c^{(i)}, \lambda^{(i)}] = \frac{1}{2} \lim_{a \to 0} \frac{\partial^2}{\partial a^2} \mathcal{L}^{(i)}[T^{(i-1)}(a), T^{(i)}(a), C^{(i)}(\mathbf{x}, t; a), \Lambda^{(i)}(\mathbf{x}, t; a)]. \tag{102}
$$

Equation (102) defines the second variation of the Lagrangian on the i^{th} interval, and is applied to (100). Suppressing the arguments of the functions $Q^{(i)}$, $C^{(i)}$, $\Lambda^{(i)}$, and $T^{(i)}$, and the superscripts on $C^{(i)}$ and $\Lambda^{(i)}$ (except when more than one interval is considered) we have

$$
\begin{aligned}
\delta^2 \mathcal{L}^{(i)}[Q^{(i)}, c^{(i)}, \lambda^{(i)}] = \frac{1}{2} \lim_{a \to 0} \frac{\partial^2}{\partial a^2} \Bigg\{ & \int_{T^{(i-1)}}^{T^{(i)}} \int_{\Gamma_1} f(t, Q^{(i)}, C, C_t) ds_1 dt \\
& + \int_{T^{(i-1)}}^{T^{(i)}} \int_{\Omega} \Lambda \left(L^{(i)} C - C_t + a_0 + Ae^{-\alpha t} \int_0^t C(\mathbf{x}, \tau; a) e^{\alpha \tau} d\tau \right) d\mathbf{x} dt \Bigg\}.
\end{aligned}
\tag{103}
$$

Notice, in (103) that the integral inside the second term above can be written as

$$
\int_0^t C(\mathbf{x}, \tau; a) e^{\alpha \tau} d\tau = \int_0^{T^{(1)}} C^{(1)}(\mathbf{x}, \tau; a) e^{\alpha \tau} d\tau + \cdots + \int_{T^{(i-1)}}^t C^{(i)}(\mathbf{x}, \tau; a) e^{\alpha \tau} d\tau \tag{104}
$$

for $i > 1$ and $t \in [T^{(i-1)}, T^{(i)}]$, where the superscript on C indicates the interval. Using Leibnitz's rule in (103) and (104) yields

$$
\begin{aligned}
&\delta^2 \mathcal{L}^{(i)}[Q^{(i)}, c^{(i)}, \lambda^{(i)}] = \\
&\quad \frac{1}{2}\lim_{a\to 0}\frac{\partial}{\partial a}\left\{\int_{T^{(i-1)}}^{T^{(i)}}\int_{\Gamma_1}(f_c C_a + f_{c_t} C_{ta})ds_1 dt + \int_{\Gamma_1} f\Big|_{t=T^{(i)}} ds_1 T_a^{(i)} - \int_{\Gamma_1} f\Big|_{t=T^{(i-1)}} ds_1 T_a^{(i-1)}\right. \\
&\quad + \int_{T^{(i-1)}}^{T^{(i)}}\int_{\Omega}\left(\begin{array}{l}\Lambda_a\left[L^{(i)}C - C_t + a_0 + Ae^{-\alpha t}\int_0^t C(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau\right] \\ +\Lambda\left[\begin{array}{l} L^{(i)}C_a - C_{ta} + Ae^{-\alpha t}\int_0^t C_a(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau + \\ C^{(1)}(\mathbf{x},T^{(1)}(a);a)e^{\alpha T^{(1)}}T_a^{(1)} + \cdots - C^{(i)}(\mathbf{x},T^{(i-1)}(a);a)e^{\alpha T^{(i-1)}}T_a^{(i-1)}\end{array}\right]\end{array}\right)dxdt \\
&\quad + \int_{\Omega}\left(\Lambda\left[L^{(i)}C - C_t + a_0 + Ae^{-\alpha t}\int_0^t C(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau\right]\right)\Big|_{t=T^{(i)}} dx T_a^{(i)} \\
&\quad \left. - \int_{\Omega}\left(\Lambda\left[L^{(i)}C - C_t + a_0 + Ae^{-\alpha t}\int_0^t C(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau\right]\right)\Big|_{t=T^{(i-1)}} dx T_a^{(i-1)}\right\}.
\end{aligned}
\tag{105}
$$

Before taking the next derivative, we examine the term

$$C^{(1)}(\mathbf{x},T^{(1)}(a);a)e^{\alpha T^{(1)}}T_a^{(1)} + \cdots - C^{(i)}(\mathbf{x},T^{(i-1)}(a);a)e^{\alpha T^{(i-1)}}T_a^{(i-1)}.$$

This term occurs from applying Leibnitz's rule for $i > 1$, since the endpoints of each interval depends on the parameter, a. When $i = 1$, this term does not appear, since the endpoints are independent of the parameter, a. In the limit (as $a \to 0$), the expression above approaches zero because of the continuity of c at each t_i. Additionally, since $h(\mathbf{x},t)$ must be as continuous as $c(\mathbf{x},t)$, then the following expression, which arises from the second derivative, approaches zero in the limit as well

$$C_a^{(1)}(\mathbf{x},T^{(1)}(a);a)e^{\alpha T^{(1)}}T_a^{(1)} + \cdots - C_a^{(i)}(\mathbf{x},T^{(i-1)}(a);a)e^{\alpha T^{(i-1)}}T_a^{(i-1)}.$$

Thus, in finding the next derivative for the second variation, these terms were omitted and the second variation could be written as

$$
\begin{aligned}
&\delta^2 \mathcal{L}^{(i)}[Q^{(i)}, c^{(i)}, \lambda^{(i)}] = \\
&\quad \frac{1}{2}\lim_{a\to 0}\Bigg\{ \int_{T^{(i-1)}}^{T^{(i)}} \int_{\Gamma_1} (f_{cc}C_a^2 + 2f_{cc_t}C_aC_{ta} + f_{c_tc_t}C_{ta}^2)ds_1dt \\
&\qquad + \int_{\Gamma_1} (f_cC_a + f_{c_t}C_{ta} + f_tT_a^{(i)} + f_c\mathcal{C}_a + f_{c_t}\mathcal{C}'_a)\Big|_{t=T^{(i)}} ds_1 T_a^{(i)} \\
&\qquad - \int_{\Gamma_1} (f_cC_a + f_{c_t}C_{ta} + f_tT_a^{(i-1)} + f_c\mathcal{C}_a + f_{c_t}\mathcal{C}'_a)\Big|_{t=T^{(i-1)}} ds_1 T_a^{(i-1)} \\
&\qquad + \int_{T^{(i-1)}}^{T^{(i)}} \int_{\Omega} 2\Lambda_a\left[L^{(i)}C_a - C_{ta} + Ae^{-\alpha t}\int_0^t C_a(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau\right]d\mathbf{x}dt \\
&\qquad + \int_{\Omega}\left(\begin{aligned}&\Lambda_a\left[L^{(i)}C - C_t + a_0 + Ae^{-\alpha t}\int_0^t C(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau\right] \\ &+\Lambda\left[L^{(i)}C_a - C_{ta} + Ae^{-\alpha t}\int_0^t C_a(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau\right]\end{aligned}\right)\Bigg|_{t=T^{(i)}} d\mathbf{x}T_a^{(i)} \\
&\qquad - \int_{\Omega}\left(\begin{aligned}&\Lambda_a\left[L^{(i)}C - C_t + a_0 + Ae^{-\alpha t}\int_0^t C(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau\right] \\ &+\Lambda\left[L^{(i)}C_a - C_{ta} + Ae^{-\alpha t}\int_0^t C_a(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau\right]\end{aligned}\right)\Bigg|_{t=T^{(i-1)}} d\mathbf{x}T_a^{(i-1)} \\
&\quad + \int_{\Omega}\left(\begin{aligned}&\Psi_a\left[L^{(i)}C - C_t + a_0 + Ae^{-\alpha t}\int_0^t C(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau\right] \\ &+\Lambda\left[\begin{aligned}&L^{(i)}\mathcal{C}_a^{(i)} - \mathcal{C}_a'^{(i)} + \frac{\partial a_0}{\partial t}T_a^{(i)} \\ &+A\left(e^{-\alpha t}\left[\int_0^t C_a(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau + Ce^{\alpha t}T_a^{(i)}\right] - \alpha e^{-\alpha t}T_a^{(i)}\int_0^t C(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau\right)\end{aligned}\right]\end{aligned}\right)\Bigg|_{t=T^{(i)}} d\mathbf{x}T_a^{(i)} \\
&\quad - \int_{\Omega}\left(\begin{aligned}&\Psi_a\left[L^{(i)}C - C_t + a_0 + Ae^{-\alpha t}\int_0^t C(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau\right] \\ &+\Lambda\left[\begin{aligned}&L^{(i)}\mathcal{C}_a^{(i)} - \mathcal{C}_a'^{(i)} + \frac{\partial a_0}{\partial t}T_a^{(i-1)} \\ &+A\left(\begin{aligned}&e^{-\alpha t}\left[\int_0^t C_a(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau + Ce^{\alpha t}T_a^{(i-1)}\right] \\ &\qquad - \alpha e^{-\alpha t}T_a^{(i-1)}\int_0^t C(\mathbf{x},\tau;a)e^{\alpha\tau}d\tau\end{aligned}\right)\end{aligned}\right]\end{aligned}\right)\Bigg|_{t=T^{(i-1)}} d\mathbf{x}T_a^{(i-1)} \Bigg\},
\end{aligned} \tag{106}
$$

where we have reintroduced the terms in (55) and defined $\mathcal{C}'^{(i)}(\mathbf{x},a) = C_t(\mathbf{x},T^{(i)}(a);a)$ for each i = 0, 1, ... n. Note also, with this definition we have

$$\mathcal{C}'^{(i)}_a = C_{tt}T^{(i)}_a + C_{ta} \tag{107}$$

This leads to the definition

$$\delta c'_i(\mathbf{x}) = \lim_{a\to 0}\mathcal{C}'^{(i)}_a(\mathbf{x},a), \tag{108}$$

where $\delta c'_i(\mathbf{x})$ is the variation in $c_t(\mathbf{x},t)$ due to the variable endpoints, t_i. From (58), (107) and (108) we see that

$$h_t(\mathbf{x},t_i) = \delta c'_i(\mathbf{x}) - c_{tt}(\mathbf{x},t_i)\Delta t_i \qquad \forall i = 0,\ 1,\ \dots\ n. \tag{109}$$

Also, since t_0 and t_n are fixed, then $\delta c'_0(\mathbf{x}) = h_t(\mathbf{x}, 0)$ and $\delta c'_n(\mathbf{x}) = h_t(\mathbf{x}, t_f)$.

Proceeding as we did with the first variation, we assume the integral is continuous on the i$^{\text{th}}$ interval and integrate by parts (over t) on the term above which includes C_t, but only on the boundary integral term

$$\int_{T^{(i-1)}}^{T^{(i)}}\int_{\Gamma_1} 2f_{cc_t}C_aC_{ta}\,ds_1dt = \int_{\Gamma_1} f_{cc_t}C_a^2\Big|_{t=T^{(i-1)}}^{t=T^{(i)}}ds_1 - \int_{T^{(i-1)}}^{T^{(i)}}\int_{\Gamma_1} C_a^2\frac{\partial}{\partial t}f_{cc_t}\,ds_1dt. \tag{110}$$

Introducing (107), (108) and (110) into (106) and letting $a \to 0$ yields for the second variation

$$
\begin{aligned}
&\delta^2\mathcal{L}^{(i)}[Q^{(i)},c^{(i)},\lambda^{(i)}] = \\
&\frac{1}{2}\Bigg\{\int_{t_{i-1}}^{t_i}\int_{\Gamma_1}\left(f_{c_tc_t}h_t^2(s,t)+\left[f_{cc}-\frac{\partial}{\partial t}f_{cc_t}\right]h^2(s,t)\right)ds_1dt \\
&+\int_{\Gamma_1}\left(\left[f_t-f_cc_t-f_{c_t}c_{tt}+f_{cc_t}c_t^2\right]\Delta t_i^2+2\left[f_c-f_{cc_t}c_t\right]\delta c_i\Delta t_i+2f_{c_t}\delta c_i'\Delta t_i+f_{cc_t}\delta c_i^2\right)\Big|_{t=t_i}ds_1 \\
&-\int_{\Gamma_1}\left(\left[f_t-f_cc_t-f_{c_t}c_{tt}+f_{cc_t}c_t^2\right]\Delta t_{i-1}^2+2\left[f_c-f_{cc_t}c_t\right]\delta c_{i-1}\Delta t_{i-1}+2f_{c_t}\delta c_{i-1}'\Delta t_{i-1}+f_{cc_t}\delta c_{i-1}^2\right)\Big|_{t=t_{i-1}}ds_1 \\
&+\int_{t_{i-1}}^{t_i}\int_\Omega 2\mu\left[L^{(i)}h-h_t+Ae^{-\alpha t}\int_0^t h(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right]d\mathbf{x}dt \\
&+\int_\Omega\left(\begin{aligned}&(\delta\lambda_i-\lambda_t\Delta t_i)\left[L^{(i)}c-c_t+a_0+Ae^{-\alpha t}\int_0^t c(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right]\\ &+\lambda\left[L^{(i)}(\delta c_i-c_t\Delta t_i)-(\delta c_i'-c_{tt}\Delta t_i)+Ae^{-\alpha t}\int_0^t h(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right]\end{aligned}\right)\Bigg|_{t=t_i}d\mathbf{x}\Delta t_i \qquad (111)\\
&-\int_\Omega\left(\begin{aligned}&(\delta\lambda_{i-1}-\lambda_t\Delta t_{i-1})\left[L^{(i)}c-c_t+a_0+Ae^{-\alpha t}\int_0^t c(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right]\\ &+\lambda\left[L^{(i)}(\delta c_{i-1}-c_t\Delta t_{i-1})-(\delta c_{i-1}'-c_{tt}\Delta t_{i-1})+Ae^{-\alpha t}\int_0^t h(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right]\end{aligned}\right)\Bigg|_{t=t_{i-1}}d\mathbf{x}\Delta t_{i-1} \\
&+\int_\Omega\left(\begin{aligned}&\delta\lambda_i\left[L^{(i)}c-c_t+a_0+Ae^{-\alpha t}\int_0^t c(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right]\\ &+\lambda\left[\begin{aligned}&L^{(i)}\delta c_i-\delta c_i'+\frac{\partial a_0}{\partial t}\Delta t_i\\ &+A\left[e^{-\alpha t}\left(\int_0^t h(\mathbf{x},\tau)e^{\alpha\tau}d\tau+ce^{\alpha t}\Delta t_i\right)-\alpha e^{-\alpha t}\Delta t_i\int_0^t c(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right]\end{aligned}\right]\end{aligned}\right)\Bigg|_{t=t_i}d\mathbf{x}\Delta t_i \\
&-\int_\Omega\left(\begin{aligned}&\delta\lambda_{i-1}\left[L^{(i)}c-c_t+a_0+Ae^{-\alpha t}\int_0^t c(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right]\\ &+\lambda\left[\begin{aligned}&L^{(i)}\delta c_{i-1}-\delta c_{i-1}'+\frac{\partial a_0}{\partial t}\Delta t_{i-1}\\ &+A\left[e^{-\alpha t}\left(\int_0^t h(\mathbf{x},\tau)e^{\alpha\tau}d\tau+ce^{\alpha t}\Delta t_{i-1}\right)-\alpha e^{-\alpha t}\Delta t_{i-1}\int_0^t c(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right]\end{aligned}\right]\end{aligned}\right)\Bigg|_{t=t_{i-1}}d\mathbf{x}\Delta t_{i-1}\Bigg\}.
\end{aligned}
$$

The equation in (111) is the second variation of the Lagrangian on the i^{th} interval, for all i = 1, 2, ... n. Again, since t_0 and t_n are fixed, we know that $\Delta t_0 = \Delta t_n = 0$. Thus, using (99) we find the second variation of the Lagrangian is the sum of a boundary

integral over all time, an integral over the domain of the aquifer over all time, and a sum of jumps at the corners, t_i

$$
\begin{aligned}
&2\delta^2 \mathcal{L}[Q, c, \lambda; \Delta t_i, h, \mu] = \\
&\quad \int_0^{t_f} \int_{\Gamma_1} \left(f_{c_t c_t} h_t^2(s,t) + \left[f_{cc} - \frac{\partial}{\partial t} f_{cc_t} \right] h^2(s,t) \right) ds_1 dt + \int_{\Gamma_1} f_{cc_t} h^2 \Big|_{t=t_f} ds_1 \qquad (112) \\
&\quad + \int_0^{t_f} \int_\Omega 2\mu \left[Lh - h_t + Ae^{-\alpha t} \int_0^t h(\mathbf{x},\tau) e^{\alpha\tau} d\tau \right] d\mathbf{x} dt \\
&+ \sum_{i=1}^{n-1} \left\{ \begin{array}{l} \displaystyle\int_{\Gamma_1} \left(\left[f_t - f_c c_t - f_{c_t} c_{tt} + f_{cc_t} c_t^2 \right] \Delta t_i^2 + 2\left[f_c - f_{cc_t} c_t \right] \delta c_i \Delta t_i + 2 f_{c_t} \delta c_i' \Delta t_i + f_{cc_t} \delta c_i^2 \right) \Big|_{t_i+0}^{t_i-0} ds_1 \\
\displaystyle + \int_\Omega \left(\begin{array}{l} \left(2\delta\lambda_i - \lambda_t \Delta t_i \right) \left[Lc - c_t + a_0 + Ae^{-\alpha t} \int_0^t c(\mathbf{x},\tau) e^{\alpha\tau} d\tau \right] \Delta t_i \\
+ 2\lambda \left[L\left(\delta c_i - c_t \Delta t_i \right) - \left(\delta c_i' - c_{tt} \Delta t_i \right) + Ae^{-\alpha t} \int_0^t h(\mathbf{x},\tau) e^{\alpha\tau} d\tau \right] \Delta t_i \\
+ \lambda \left[Lc_t - c_{tt} + \dfrac{\partial a_0}{\partial t} + A\left(c - \alpha e^{-\alpha t} \int_0^t c(\mathbf{x},\tau) e^{\alpha\tau} d\tau \right) \right] \Delta t_i^2 \end{array} \right) \Bigg|_{t_i+0}^{t_i-0} d\mathbf{x} \end{array} \right\}.
\end{aligned}
$$

To simplify equation (112), we assume that c is sufficiently differentiable, so that the last term in the integral on Ω can be written as

$$
\begin{aligned}
&\lambda \left[Lc_t - c_{tt} + \frac{\partial a_0}{\partial t} + A\left(c - \alpha e^{-\alpha t} \int_0^t c(\mathbf{x},\tau) e^{\alpha\tau} d\tau \right) \right] \\
&\qquad\qquad = \lambda \frac{\partial}{\partial t} \left[Lc - c_t + a_0 + Ae^{-\alpha t} \int_0^t c(\mathbf{x},\tau) e^{\alpha\tau} d\tau \right]. \qquad (113)
\end{aligned}
$$

Also, recall that the operator L depends on the status of the pump so that $L\big|_{t_i-0} = L^{(i)}$ and $L\big|_{t_i+0} = L^{(i+1)}$. Substituting (113) into (112) the second variation becomes

$$
\begin{aligned}
&2\delta^2 \mathcal{L}[Q, c, \lambda; \Delta t_i, h, \mu] = \\
&\quad \int_0^{t_f} \int_{\Gamma_1} \left(f_{c_t c_t} h_t^2(s,t) + \left[f_{cc} - \frac{\partial}{\partial t} f_{cc_t} \right] h^2(s,t) \right) ds_1 dt + \int_{\Gamma_1} f_{cc_t} h^2 \Big|_{t=t_f} ds_1 \qquad (114) \\
&\qquad + \int_0^{t_f} \int_{\Omega} 2\mu \left[Lh - h_t + Ae^{-\alpha t} \int_0^t h(\mathbf{x},\tau) e^{\alpha\tau} d\tau \right] d\mathbf{x} dt \\
&+ \sum_{i=1}^{n-1} \left\{ \begin{array}{l} \displaystyle \int_{\Gamma_1} \left(\left[f_t - f_c c_t - f_{c_t} c_{tt} + f_{cc_t} c_t^2 \right] \Delta t_i^2 + 2\left[f_c - f_{cc_t} c_t \right] \delta c_i \Delta t_i + 2 f_{c_t} \delta c_i' \Delta t_i + f_{cc_t} \delta c_i^2 \right) \Big|_{t_i+0}^{t_i-0} ds_1 \\ \displaystyle + \int_{\Omega} \left(\begin{array}{l} \left(2\delta\lambda_i - \lambda_t \Delta t_i + \lambda \Delta t_i \frac{\partial}{\partial t} \right) \cdot \left[Lc - c_t + a_0 + Ae^{-\alpha t} \int_0^t c(\mathbf{x},\tau) e^{\alpha\tau} d\tau \right] \Delta t_i \\ + 2\lambda \left[L(\delta c_i - c_t \Delta t_i) - (\delta c_i' - c_{tt} \Delta t_i) + Ae^{-\alpha t} \int_0^t h(\mathbf{x},\tau) e^{\alpha\tau} d\tau \right] \Delta t_i \end{array} \right) \Bigg|_{t_i+0}^{t_i-0} d\mathbf{x} \end{array} \right\}.
\end{aligned}
$$

Equation (114) is the form of the second variation of the Lagrangian that was used to derive necessary conditions for a minimal solution. The next section presents a theorem which is proven by a thorough investigation of the admissible variations of h, μ, Δt_i, δc_i, $\delta c_i'$, and $\delta\lambda_i$. This proof establishes a set of NOCs which must be satisfied by a minimal solution of the optimization problem described in Chapter III.

5.2 *Admissible Variations*

The preceding section developed the second variation of the Lagrangian for the functional in (24) constrained by the conditions in (25) - (27). The present section analyzes the second variation, applying the theory stated in the Chapter III to arrive at NOCs for the existence of an optimal pulsed pumping schedule. In this section, we will investigate equation (114) and prove a necessary conditions theorem by examining the sets of admissible variations of c, λ, and t_i. Again, as in the case for the admissible variation of the first variation of the Lagrangian, examination of special cases led to

necessary conditions that must be met for all points within the aquifer. Before proceeding with this investigation, we present two lemmas which aid in the discussion.

Lemma 4. Suppose P and Q are both continuous on [a, b]. A necessary condition for the quadratic functional

$$A[h]=\int_a^b [P(x)h'^2(x)+Q(x)h^2(x)]dx$$

defined for all functions $h\in C^1(a,b)$ such that $h(a) = h(b) = 0$, to be nonnegative is that

$$P(x)\geq 0 \qquad (a\leq x\leq b)$$

(Gelfand & Fomin, 1963:103).

The following lemma is similar to Lemma 4:

Lemma 5. Suppose that $P(x) \geq 0$ and Q are both continuous for all $x \in [a,c) \cup (c,b]$ and m is a constant, a necessary condition for the quadratic functional

$$A(x)=\int_a^b [P(x)h'^2(x)+Q(x)h^2(x)]dx+mh^2(c)$$

defined for all $h\in C^1(a,b)$ such that $h(a) = h(b) = 0$, to be nonnegative is that

$$m+\min\left\{\lim_{x\to c^-} P(x), \lim_{x\to c^+} P(x)\right\}\geq 0 \qquad (a<c<b).$$

Proof. This proof is similar to the proof of Lemma 4 presented by Gelfand & Fomin (1963). Without loss of generality, suppose $\lim_{x\to c^-} P(x)$ is the minimum of the two one-sided limits and also suppose the inequality above does not hold. That is, suppose $m + \lim_{x\to c^-} P(x) = -2\beta$ $(\beta > 0)$. If P(x) is continuous on [a, c), then there exists $\alpha > 0$ where

$$P(x)+m<-\beta \qquad \forall x\in (c-\alpha,c].$$

Now, choose $h \in C^1(a, b)$ such that the quadratic functional A is negative. That is, let

$$h(x) = \begin{cases} \sin^2\left[\pi\left(\dfrac{x-c}{2\alpha}\right) + \dfrac{\pi}{2}\right] & c-\alpha \le x \le c \\ 0 & \text{otherwise.} \end{cases}$$

Then we have

$$\begin{aligned} \int_a^b [P(x)h'^2(x) + Q(x)h^2(x)]dx + mh^2(c) &= \int_{c-\alpha}^{c} P(x)\frac{\pi^2}{4\alpha^2}\sin^2\left[\frac{\pi(x-c)}{\alpha}\right]dx \\ &+ \int_{c-\alpha}^{c} Q(x)\frac{\pi^2}{4\alpha^2}\sin^4\left[\frac{\pi(x-c)}{2\alpha} + \frac{\pi}{2}\right]dx + m \\ &< -(\beta + m)\frac{\pi^2}{4\alpha^2}\cdot\alpha + M\alpha + m \end{aligned}$$

where $M = \max_{a \le x \le b} |Q(x)|$. For sufficiently small α, the right-hand side of this equation becomes negative. This contradiction proves the lemma. □

We now state a theorem which provides necessary conditions for the second variation to produce a minimum for the optimization problem of Chapter III.

Theorem 7. (Necessary Optimality Conditions of the Second Variation) Let J[Q,c] be the functional given by equation (24), constrained by the boundary value problem defined by equations (25) through (27), and assume that f has continuous first and second partial derivatives for all of its arguments on the i^{th} interval of $[0, t_f]$, given as $[t_{i-1}, t_i]$ for all $i = 1, 2, \ldots n$. Let $c(\mathbf{x},t)$ and $\lambda(\mathbf{x},t)$ be given as $c(\mathbf{x},t) = c^{(i)}(\mathbf{x},t)$ and $\lambda(\mathbf{x},t) = \lambda^{(i)}(\mathbf{x},t)$, and let $Q(t) = Q^{(i)}(t)$, (defined by equation (43)) for $t \in [t_{i-1}, t_i]$ and for all $i = 1, 2, \ldots n$. If the functions $(\hat{Q}, \hat{c}, \hat{\lambda})$ produce a minimum for the functional in (24) constrained by (25) through (27), then the following conditions are necessary

$$f_{c_t c_t}[t, \hat{Q}^{(i)}(t), \hat{c}^{(i)}(\mathbf{x}_w t), \hat{c}_t^{(i)}(\mathbf{x}_w t)] \ge 0$$

for all $t \in [t_{i-1}, t_i]$, and for all $i = 1, 2, \ldots n$,

$$\det \mathbf{M}^{(i)} \geq 0,$$

for all $i = 1, 2, \ldots n-1$, where $\mathbf{M}^{(i)}$ is given as

$$\mathbf{M}^{(i)} = \frac{1}{2}\begin{bmatrix} \left(\hat{f}_t - \hat{f}_c \hat{c}_t - \hat{f}_{c_t} \hat{c}_{tt} + \hat{f}_{cc_t} \hat{c}_t^2\right)\Big|_{t_i+0}^{t_i-0} & \left(\hat{f}_c - \hat{f}_{cc_t} \hat{c}_t\right)\Big|_{t_i+0}^{t_i-0} \\ \left(\hat{f}_c - \hat{f}_{cc_t} \hat{c}_t\right)\Big|_{t_i+0}^{t_i-0} & \hat{f}_{cc_t}\Big|_{t_i+0}^{t_i-0} \end{bmatrix}_{\mathbf{x}=\mathbf{x}_w}$$

and

$$\left[\hat{f}_t - \hat{f}_c \hat{c}_t - \hat{f}_{c_t} \hat{c}_{tt} + \hat{f}_{cc_t} \hat{c}_t^2\right]_{\mathbf{x}=\mathbf{x}_w}\Big|_{t_i+0}^{t_i-0} \geq 0$$

$$\left[\hat{f}_{cc_t}\right]_{\mathbf{x}=\mathbf{x}_w}\Big|_{t_i+0}^{t_i-0} > 0$$

for all $i = 1, 2, \ldots n-1$. For a maximum, the signs $\geq$ and $>$ are replaced by $\leq$ and $<$, respectively.

Proof. In this proof, we establish necessary conditions for the existence of a minimum solution for the functional in (24), constrained by (25) through (27). Suppose the functions $(\hat{Q}, \hat{c}, \hat{\lambda})$ represent a minimum solution for this optimization problem, then the NOCs of Theorem 6 must hold for $(\hat{Q}, \hat{c}, \hat{\lambda})$. Specifically, NOCs (83a), (84a), and (89), restated here as

$$\hat{f}_{c_t}\Big|_{t_i+0}^{t_i-0} = 0 \qquad \forall \mathbf{x} \in \Gamma_1 \text{ and } \forall i = 1, 2, \ldots n-1,$$

$$\hat{f}_{c_t}\Big|_{t=t_f} = 0 \qquad \forall \mathbf{x} \in \Gamma_1,$$

and

$$L\hat{c} + a_0 - \hat{c}_t + Ae^{-\alpha t}\int_0^t \hat{c}(\mathbf{x},\tau)e^{\alpha\tau}d\tau = 0 \qquad \forall\ (\mathbf{x},t) \in \Omega \times [t_{i-1}, t_i]$$

must hold for the optimal solution, reducing equation (114) to

$$
\begin{aligned}
2\delta^2 \mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i, h, \mu] = & \\
& \int_0^{t_f}\int_{\Gamma_1}\left(\hat{f}_{c_t c_t} h_t^2(s,t) + \left[\hat{f}_{cc} - \frac{\partial}{\partial t}\hat{f}_{cc_t}\right] h^2(s,t)\right) ds_1 dt \\
& + \int_0^{t_f}\int_{\Omega} 2\mu\left[Lh - h_t + Ae^{-\alpha t}\int_0^t h(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right] d\mathbf{x}dt \\
+\sum_{i=1}^{n-1} & \left\{
\begin{aligned}
&\int_{\Gamma_1}\left(\left[\hat{f}_t - \hat{f}_c\hat{c}_t - \hat{f}_{c_t}\hat{c}_{tt} + \hat{f}_{cc_t}\hat{c}_t^2\right]\Delta t_i^2 + 2\left[\hat{f}_c - \hat{f}_{cc_t}\hat{c}_t\right]\delta c_i \Delta t_i + \hat{f}_{cc_t}\delta c_i^2\right)\Big|_{t_i+0}^{t_i-0} ds_1 \\
&+\int_{\Omega}\left(2\hat{\lambda}\left[L(\delta c_i - \hat{c}_t\Delta t_i) - (\delta c_i' - \hat{c}_{tt}\Delta t_i) + Ae^{-\alpha t}\int_0^t h(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right]\Delta t_i\right)\Big|_{t_i+0}^{t_i-0} d\mathbf{x}
\end{aligned}
\right\}.
\end{aligned}
\tag{115}
$$

In the rest of this proof, we examine (115) looking at all possibilities for the variations of c, λ, and t_i. In analyzing the first variation, we found conditions on terms that must vanish for all space and time depending on whether the point in space was on the domain or the boundary of the aquifer. These conditions were then applied to the first variation, simplifying the expression with each new necessary condition, until finally all necessary conditions were found that guaranteed the first variation would vanish, as required by Theorem 1.

In the case of the second variation, Theorem 3 makes it necessary for the second variation to be nonnegative for the existence of a minimum solution. Thus, each new necessary condition does not always reduce the second variation, and the analysis is somewhat different from what was presented in Chapter IV. The remainder of this proof presents an itemized account of admissible variations which led to necessary conditions for the second variation of the Lagrangian.

Case 1. First, suppose the pump switching times are fixed; $\Delta t_i = 0$ for all i = 1, 2, ... n-1, reducing the second variation for optimal $(\hat{Q}, \hat{c}, \hat{\lambda})$ in (115) to

$$2\delta^2 \mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i = 0, h, \mu] = \int_0^{t_f}\int_{\Gamma_1}\left(\hat{f}_{c_t c_t} h_t^2(s,t) + \left[\hat{f}_{cc} - \frac{\partial}{\partial t}\hat{f}_{cc_t}\right] h^2(s,t)\right) ds_1 dt + \sum_{i=1}^{n-1}\int_{\Gamma_1}\hat{f}_{cc_t} h^2(s,t)\Big|_{t_i+0}^{t_i-0} ds_1 + \int_0^{t_f}\int_{\Omega} 2\mu\left[Lh - h_t + Ae^{-\alpha t}\int_0^t h(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right]d\mathbf{x}dt \qquad (116)$$

Next, subcases of this first case were examined to investigate all possibilities for $h \in H$, the set of admissible variations of the concentration, and for $\mu \in M$, the set of admissible variations of the Lagrange multiplier. The first assumption is that admissible h is nonzero on a single sub-interval of $[0, t_f]$. Let $i \in \{1, 2, \ldots n\}$ be fixed and suppose h is nonzero on the i^{th} interval only, that is, $h \neq 0$ for all $t \in (t_{i-1}, t_i)$ and for all $\mathbf{x} \in \Omega \cup \Gamma$. To establish necessary conditions for the second variation, we must satisfy $\delta^2 \mathcal{L} \geq 0$, given that $\delta\mathcal{L} = 0$, for the case defined above on every interval of $[0, t_f]$.

(a) Initially, choose $h(\mathbf{x}, t)$ such that

(i) $h(\mathbf{x}, t) = 0 \quad \forall\, \mathbf{x} \in \Omega \cup \Gamma$ and $\forall\, t \notin (t_{i-1}, t_i)$

(ii) $h(\mathbf{x}, t) = 0 \quad \forall\, \mathbf{x} \in \Gamma = \Gamma_1 \cup \Gamma_2$ and $\forall\, t \in [t_{i-1}, t_i]$.

This choice of $h(\mathbf{x}, t)$ is identical to case 1(a) in Theorem 6, so that Figure 6 applies again here. Applying (i) and (ii) above to (116), we have

$$2\delta^2 \mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};0,h,\mu] = \int_{t_{i-1}}^{t_i}\int_{\Omega} 2\mu\left[L^{(i)}h - h_t + Ae^{-\alpha t}\int_0^t h(\mathbf{x},\tau)e^{\alpha\tau}d\tau\right]d\mathbf{x}dt \qquad (117)$$

If $\mu(\mathbf{x}, t) = 0$ for all $\mathbf{x} \in \Omega$ and $t \in [0, t_n]$, then $\delta^2 \mathcal{L}^{(i)} = 0$ and the second variation of the Lagrangian is nonnegative, as required. Now, suppose $\mu(\mathbf{x}, t) \neq 0$ for all $\mathbf{x} \in \Omega$ and $t \in (t_{i-1}, t_i)$ and $\mu(\mathbf{x}, t) = 0$ for all $\mathbf{x} \in \Omega$ and $t \in [0, t_{i-1}] \cup [t_i, t_n]$ (that is, $\mu(\mathbf{x}, t) \neq 0$ on the i^{th} interval only). Further, suppose $h(\mathbf{x}, t)$ is <u>fixed</u> such that

$$L^{(i)}h - h_t + Ae^{-\alpha t} \int_0^t h(\mathbf{x}, \tau) e^{\alpha \tau} d\tau \geq 0$$

for all $\mu \in M$, the set of admissible variations of λ. If $\mu \in M$ such that $\mu > 0$ then $\delta^2 \mathcal{L}^{(i)} \geq 0$. However, if $\mu \in M$ such that $\mu < 0$ then $\delta^2 \mathcal{L}^{(i)} \leq 0$. Since we cannot have both, then we must have $\delta^2 \mathcal{L}^{(i)} = 0$. Since $\mu(\mathbf{x}, t) \neq 0$, then

$$L^{(i)}h - h_t + Ae^{-\alpha t} \int_0^t h(\mathbf{x}, \tau) e^{\alpha \tau} d\tau = 0 \tag{118}$$

is necessary for all $\mathbf{x} \in \Omega$, $t \in (t_{i-1}, t_i)$ and for all $i = 1, 2, \ldots n$. On <u>any given interval</u>, (t_{i-1}, t_i), the integro-differential operator defined by (118) is a continuous, linear operator. Since (118) must hold for every interval, and since $h(\mathbf{x}, t)$ is also continuous, then (118) must also hold at the endpoints of each interval. That is

$$Lh(\mathbf{x}, t_i) - h_t(\mathbf{x}, t_i) + Ae^{-\alpha t_i} \int_0^{t_i} h(\mathbf{x}, \tau) e^{\alpha \tau} d\tau = 0 \tag{119}$$

for any $i = 1, 2, \ldots n-1$, is necessary. Recalling equations (58) which defined $h(\mathbf{x}, t_i)$ and equation (109) which defined $h_t(\mathbf{x}, t_i)$, then (118) and (119) applied to (115) reduces the second variation of the Lagrangian to

$$
\begin{aligned}
&2\delta^2 \mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i, h, \mu] = \\
&\int_0^{t_f}\int_{\Gamma_1}\left(\hat{f}_{c_t c_t} h_t^2(s,t) + \left[\hat{f}_{cc} - \frac{\partial}{\partial t}\hat{f}_{cc_t}\right] h^2(s,t)\right) ds_1 dt \\
&+ \sum_{i=1}^{n-1}\int_{\Gamma_1}\left(\left[\hat{f}_t - \hat{f}_c \hat{c}_t - \hat{f}_{c_t}\hat{c}_{tt} + \hat{f}_{cc_t}\hat{c}_t^2\right]\Delta t_i^2 + 2\left[\hat{f}_c - \hat{f}_{cc_t}\hat{c}_t\right]\delta c_i \Delta t_i + \hat{f}_{cc_t}\delta c_i^2\right)_{c=\hat{c}}\Big|_{t_i+0}^{t_i-0} ds_1,
\end{aligned}
\tag{120}
$$

and for Case 1, which we are presently considering (i.e., $\Delta t_i = 0$ for all $i = 1, 2, \ldots n\text{-}1$), equation (116) becomes

$$
\begin{aligned}
&2\delta^2 \mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i = 0, h, \mu] = \\
&\int_0^{t_f}\int_{\Gamma_1}\left(\hat{f}_{c_t c_t} h_t^2(s,t) + \left[\hat{f}_{cc} - \frac{\partial}{\partial t}\hat{f}_{cc_t}\right] h^2(s,t)\right) ds_1 dt + \sum_{i=1}^{n-1}\int_{\Gamma_1}\hat{f}_{cc_t} h^2(s,t)\Big|_{t_i+0}^{t_i-0} ds_1.
\end{aligned}
\tag{121}
$$

(b) Next, allow nonzero h at the well as in case 1(b) of Theorem 6. Choose $h \in H$ such that

(i) $h(\mathbf{x}, t) = 0 \quad \forall\, \mathbf{x} \in \Omega \cup \Gamma$ and $\forall\, t \notin (t_{i-1}, t_i)$

(ii) $h(\mathbf{x}, t) = 0 \quad \forall\, \mathbf{x} \in \Gamma_2$ and $\forall\, t \in [t_{i-1}, t_i]$.

With these assumptions, the second variation of the Lagrangian (121) becomes

$$
\delta^2 \mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i = 0, h, \mu] = \frac{1}{2}\int_{t_{i-1}}^{t_i}\int_{\Gamma_1}\left(\hat{f}_{c_t c_t} h_t^2(s,t) + \left[\hat{f}_{cc} - \frac{\partial}{\partial t}\hat{f}_{cc_t}\right] h^2(s,t)\right) ds_1 dt. \tag{122}
$$

Letting the boundary of the well shrink to a point (i.e., $\Gamma_1 \rightarrow 0$) and applying Lemma 4 to the functional (122), a necessary condition for (122) to be nonnegative is that

$$
f_{c_t c_t}[t, \hat{Q}^{(i)}(t), \hat{c}(\mathbf{x}_w t), \hat{c}_t(\mathbf{x}_w t)] \geq 0 \tag{123}
$$

for all $t \in [t_{i-1}, t_i]$, and for all $i = 1, 2, \ldots n$.

The necessary condition in (123) provides a tool which can be used to determine the classes of functionals in (24) which can be minimized through this variational approach. Additional necessary conditions are derived in case 2, where we allow the switching times to vary. Before pursuing this case, notice that the second variation in equation (120) contains only spatial integrations around the boundary of the well. Since the diameter of the well is small compared to the domain of the aquifer, allowing $\Gamma_1 \to 0$ allows these integrals to become evaluation of the integrand at the location of the pumping well, as we saw in Theorem 6 and above in deriving (123). Thus, letting $\Gamma_1 \to 0$, equation (120) becomes

$$
\begin{aligned}
&2\delta^2 \mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i,h,\mu] = \\
&\quad \int_0^{t_f} \left(\hat{f}_{c_t c_t} h_t^2 + \left[\hat{f}_{cc} - \frac{\partial}{\partial t}\hat{f}_{cc_t} \right] h^2 \right)_{x=x_w} dt \qquad (124) \\
&\quad + \sum_{i=1}^{n-1} \left(\left[\hat{f}_t - \hat{f}_c \hat{c}_t - \hat{f}_{c_t} \hat{c}_{tt} + \hat{f}_{cc_t} \hat{c}_t^2 \right] \Delta t_i^2 + 2\left[\hat{f}_c - \hat{f}_{cc_t} \hat{c}_t \right] \delta c_i \Delta t_i + \hat{f}_{cc_t} \delta c_i^2 \right)_{x=x_w} \Big|_{t_i+0}^{t_i-0}.
\end{aligned}
$$

Now, we define the following terms to write (124) in a compact form

$$
P^{(i)}(t) = \frac{1}{2} f_{c_t c_t}[t,\hat{Q}^{(i)}(t),\hat{c}^{(i)}(\mathbf{x}_w,t),\hat{c}_t^{(i)}(\mathbf{x}_w,t)],
$$

$$
R^{(i)}(t) = \frac{1}{2}\left\{ f_{cc}[t,\hat{Q}^{(i)}(t),\hat{c}^{(i)}(\mathbf{x}_w,t),\hat{c}_t^{(i)}(\mathbf{x}_w,t)] - \frac{\partial}{\partial t} f_{cc_t}[t,\hat{Q}^{(i)}(t),\hat{c}^{(i)}(\mathbf{x}_w,t),\hat{c}_t^{(i)}(\mathbf{x}_w,t)] \right\}, \qquad (125)
$$

$$
m_{11}^{(i)} = \frac{1}{2}\left[\hat{f}_t - \hat{f}_c \hat{c}_t - \hat{f}_{c_t} \hat{c}_{tt} + \hat{f}_{cc_t} \hat{c}_t^2 \right]_{x=x_w} \Big|_{t_i+0}^{t_i-0},
$$

$$
m_{12}^{(i)} = m_{21}^{(i)} = \frac{1}{2}\left[\hat{f}_c - \hat{f}_{cc_t} \hat{c}_t \right]_{x=x_w} \Big|_{t_i+0}^{t_i-0}, \qquad \text{and} \qquad m_{22}^{(i)} = \frac{1}{2}\left[\hat{f}_{cc_t} \right]_{x=x_w} \Big|_{t_i+0}^{t_i-0}.
$$

With these definitions, the second variation of the Lagrangian can be written as

$$\delta^2 \mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i, h, \mu] = \int_0^{t_f} \left(P(t)h_t^2(t) + R(t)h^2(t)\right)dt + \sum_{i=1}^{n-1} \begin{bmatrix} \Delta t_i & \delta c_i \end{bmatrix} \cdot \begin{bmatrix} m_{11}^{(i)} & m_{12}^{(i)} \\ m_{21}^{(i)} & m_{22}^{(i)} \end{bmatrix} \cdot \begin{bmatrix} \Delta t_i \\ \delta c_i \end{bmatrix}. \quad (126)$$

Note that the superscripts on P and R are suppressed, and understood to change on each time interval of the above integral.

The next case examines the possibility of varying the switching times while the variation of the concentration is also nonzero. Additional necessary conditions arise from this case and aid the analysis of general classes of functionals, presented in Chapter VII.

<u>**Case 2.**</u> This case establishes necessary conditions at the switching times, produced by examining the possibility of a nonzero variation of the concentration on consecutive intervals of time, (Figure 9). Suppose

(i) $h(\mathbf{x}_w, t) = 0 \qquad \forall\, t \in [0, t_{i-1}] \cup [t_{i+1}, t_f]$

(ii) $\Delta t_i \neq 0, \quad \Delta t_j = 0 \qquad \forall\, j \neq i$

(iii) $\delta c_i \neq 0, \quad \delta c_j = 0 \qquad \forall\, j \neq i.$

With these assumptions, the second variation in (126) becomes

$$\delta^2 \mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i, h, \mu] = \int_{t_{i-1}}^{t_{i+1}} \left(P(t)h_t^2 + R(t)h^2\right)dt + \begin{bmatrix} \Delta t_i & \delta c_i \end{bmatrix} \cdot \mathbf{M}^{(i)} \cdot \begin{bmatrix} \Delta t_i \\ \delta c_i \end{bmatrix}. \quad (127)$$

where $\mathbf{M}^{(i)}$ represents the matrix in (126) with elements defined by (125).

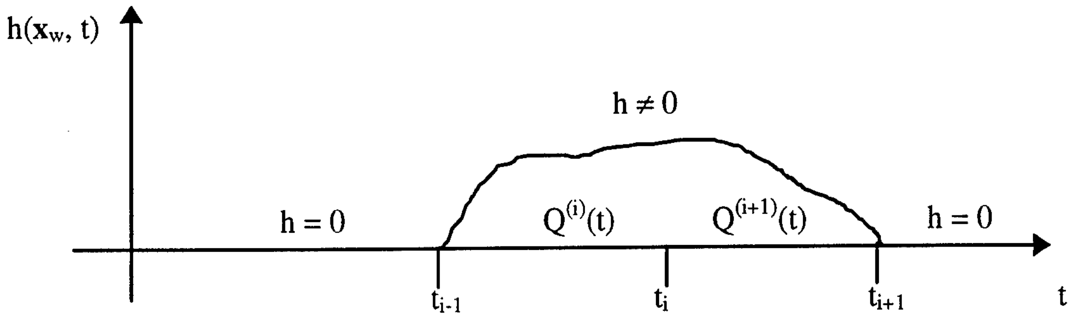

Figure 9. The variation of the concentration, $h(\mathbf{x}_w, t)$, is nonzero on consecutive intervals of $[0, t_f]$ and zero elsewhere.

The analysis of (127) requires a simplifying assumption for the relationship between δc_i and Δt_i. A linear relationship was assumed and could be justified by the choice of a specific variation h. Thus, we assume

$$\delta c_i = \mathcal{X}\Delta t_i, \tag{128}$$

where $\mathcal{X} \in \mathbf{R}$. With this linear relationship, any specific $h(\mathbf{x}_w, t_i)$ could be defined by the choice of $\mathcal{X}$. Theorem 3 requires that (127) should be nonnegative for all admissible values of h. With the choice of the relationship in (128), we need (127) to be nonnegative for any real $\mathcal{X}$. Using (128) in (127) we have (suppressing the i's on the elements of $\mathbf{M}^{(i)}$)

$$\begin{aligned} \delta^2 \mathcal{L}[\hat{Q}, \hat{c}, \hat{\lambda}; \Delta t_i, h, \mu] &= \int_{t_{i-1}}^{t_{i+1}} \left(P(t)h_t^2 + R(t)h^2\right)dt + \begin{bmatrix} 1 & \mathcal{X} \end{bmatrix} \cdot \mathbf{M}^{(i)} \cdot \begin{bmatrix} 1 \\ \mathcal{X} \end{bmatrix} \Delta t_i^2 \\ &= \int_{t_{i-1}}^{t_{i+1}} \left(P(t)h_t^2 + R(t)h^2\right)dt + \left(m_{11} + 2\mathcal{X}m_{12} + \mathcal{X}^2 m_{22}\right)\Delta t_i^2 \geq 0 \end{aligned} \tag{129}$$

for all i = 1, 2, ... n-1. Recall, from equation (58) we have

$$h(\mathbf{x}_w, t_i) = (\mathcal{X} - c_t)\Delta t_i \quad \text{which implies} \quad \Delta t_i = \frac{h(\mathbf{x}_w, t_i)}{\mathcal{X} - c_t}. \tag{130}$$

Substituting Δt_i from (130) into the inequality of (129), we have

$$\int_{t_{i-1}}^{t_{i+1}} \left(P(t)h_t^2 + R(t)h^2\right)dt + \frac{m_{11} + 2\mathcal{X}m_{12} + \mathcal{X}^2 m_{22}}{(\mathcal{X} - c_t)^2} h^2(\mathbf{x}_w, t_i) \geq 0. \tag{131}$$

Lemma 5 asserts that a necessary condition for (131) to hold is that

$$P(t_i) + \frac{m_{11} + 2\mathcal{X}m_{12} + \mathcal{X}^2 m_{22}}{(\mathcal{X} - c_t)^2} \geq 0 \qquad t_{i-1} < t_i < t_{i+1} \tag{132}$$

for all real $\mathcal{X}$, where $P(t_i) = \min\left\{\lim_{t \to t_i^-} P^{(i)}(t), \lim_{t \to t_i^+} P^{(i+1)}(t)\right\}$. In order to satisfy the inequality in (132) for all possible values of $\mathcal{X}$, we must have

$$m_{11} + 2\mathcal{X}m_{12} + \mathcal{X}^2 m_{22} \geq 0 \tag{133}$$

The left-hand side of inequality (133) represents a parabolic function $f(\mathcal{X})$, which is concave up and has at most one real root. The roots of this equation are given as

$$\mathcal{X}_{1,2} = \frac{-m_{12} \pm \sqrt{m_{12}^2 - m_{11}m_{22}}}{m_{22}}, \tag{134}$$

or we can write

$$\mathcal{X}_{1,2} = \frac{-m_{12} \pm \sqrt{-\det \mathbf{M}^{(i)}}}{m_{22}}. \tag{135}$$

To ensure (135) has at most one real root, and since i is arbitrary, we have the necessary conditions

$$\det \mathbf{M}^{(i)} \geq 0 \tag{136}$$

and

$$m_{22} > 0 \tag{137}$$

for all i = 1, 2, ... n-1. Recall, (133) is also necessary for all $\mathcal{X} \in \mathbf{R}$. Two special cases arise from examining the admissible values of $\mathcal{X}$: (a) $\mathcal{X} = 0$ and (b) $\mathcal{X} \rightarrow \pm\infty$. The first case would arise from allowing δc_i to be zero while allowing Δt_i to vary, and the second case occurs while allowing Δt_i to be zero while allowing δc_i to vary.

Case (a): If $\mathcal{X} = 0$, then (133) becomes the necessary condition

$$m_{11} \geq 0 \tag{138}$$

Case (b): If $\mathcal{X} \rightarrow \pm\infty$, then (133) implies that $m_{22} \geq 0$. But the necessary condition in (137) is stronger, so nothing more is gained here.

With the NOCs derived in the inequalities in (123), (136), (137), and (138), the theorem has been proved. □

5.3 *Summary*

This chapter developed the second variation of the Lagrangian and proved a necessary conditions theorem by examining the admissible variations h, Δt_i, and δc_i. The

analysis led to necessary conditions for a minimal solution to the optimization problem of Chapter III, which are contained in (123), (136), (137), and (138), restated here as

$$f_{c_t c_t}[t, \hat{Q}^{(i)}(t), \hat{c}^{(i)}(\mathbf{x}_w t), \hat{c}_t^{(i)}(\mathbf{x}_w t)] \geq 0 \tag{139}$$

for all $t \in [t_{i-1}, t_i]$, and for all $i = 1, 2, \ldots n$,

$$\det \mathbf{M}^{(i)} \geq 0, \tag{140}$$

$$\left[\hat{f}_t - \hat{f}_c \hat{c}_t - \hat{f}_{c_t} \hat{c}_{tt} + \hat{f}_{cc_t} \hat{c}_t^2\right]_{\mathbf{x}=\mathbf{x}_w} \Big|_{t_i+0}^{t_i-0} \geq 0, \tag{141}$$

and

$$\left[\hat{f}_{cc_t}\right]_{\mathbf{x}=\mathbf{x}_w} \Big|_{t_i+0}^{t_i-0} > 0 \tag{142}$$

for all $i = 1, 2, \ldots n\text{-}1$, where $\mathbf{M}^{(i)}$ is given as

$$\mathbf{M}^{(i)} = \frac{1}{2}\begin{bmatrix} \left(\hat{f}_t - \hat{f}_c \hat{c}_t - \hat{f}_{c_t} \hat{c}_{tt} + \hat{f}_{cc_t} \hat{c}_t^2\right)\Big|_{t_i+0}^{t_i-0} & \left(\hat{f}_c - \hat{f}_{cc_t} \hat{c}_t\right)\Big|_{t_i+0}^{t_i-0} \\ \left(\hat{f}_c - \hat{f}_{cc_t} \hat{c}_t\right)\Big|_{t_i+0}^{t_i-0} & \hat{f}_{cc_t}\Big|_{t_i+0}^{t_i-0} \end{bmatrix}_{\mathbf{x}=\mathbf{x}_w}.$$

The next chapter presents the analysis that led to sufficient conditions for a minimum solution. A theorem is presented which guarantees the quadratic functional (127) is positive definite, as required by Theorem 4, thereby establishing sufficient conditions for a minimum and leading to a sufficiency theorem that lists the conditions which are both necessary and sufficient for a minimal solution.

VI. Sufficient Optimality Conditions for a Minimum

The first and second variations of the Lagrangian have thus far provided necessary conditions which must be met by any solution that minimizes the optimization problem presented in Chapter III. That is, given that $(\hat{Q}, \hat{c}, \hat{\lambda})$ is an optimal solution, then the necessary conditions of Chapters IV and V must be satisfied by this solution to be a minimal solution. The goal of the current chapter is to establish conditions which, if satisfied, will guarantee this solution is a minimal solution. That is, given that $(\hat{Q}, \hat{c}, \hat{\lambda})$ satisfies these sufficient conditions, then the solution is, in fact, a minimal solution for the optimization problem.

As discussed in Chapter III, the theory presented in this chapter builds on the notion that the second variation of the Lagrangian must be positive definite at $(\hat{Q}, \hat{c}, \hat{\lambda})$, given that the first variation of the Lagrangian vanishes there. The first section of this chapter motivates the theorems presented in the sections that follow. Again, as in the analysis of the first and second variations, the motivation comes from the examination of the simplest variational problem (equation (31) of Chapter III), which in turn leads to both necessary and sufficient conditions for the second variation of the Lagrangian to be positive definite. The so-called *Secondary Variational Problem* is developed and analyzed in section 6.2, and the analysis leads to a definition of the important concept of a *conjugate time*. Also, this section motivates the theorems presented in the subsequent sections of the chapter which establish positive definiteness of the second variation of the

Lagrangian, as well as sufficiency conditions for a minimal solution for the optimization problem.

6.1 Motivation

In this section, we return to the simplest variational problem to establish the direction for the analysis that follows. For the case of the simplest variational problem, we seek to find an extremum for the functional in (31) which satisfies the boundary conditions in (30). Assuming that the first variation of the functional in (31) vanishes at some optimal $\hat{y}$, then the pursuit of an extremal for the functional reduces to an analysis of the second variation of (31), given by the quadratic functional

$$\int_a^b (Ph'^2 + Qh^2)dx, \tag{143}$$

defined on the set of admissible functions h(x) which satisfy the homogeneous boundary conditions $h(a) = h(b) = 0$. For this problem, the functions P and Q are related to F in (31) as

$$P = \frac{1}{2}F_{y'y'}, \qquad Q = \frac{1}{2}\left(F_{yy} - \frac{d}{dx}F_{yy'}\right). \tag{144}$$

Application of Theorem 3 to the simplest problem leads to the necessary (but not sufficient) condition that $P(x) \geq 0$, for all $x \in [a, b]$, for the quadratic functional in (143) to be ≥ 0 for all admissible variations h(x). If we assume the strengthened inequality

$$P(x) > 0, \qquad (a \leq x \leq b) \tag{145}$$

holds, we can then find conditions which are both necessary and sufficient for the second variation to be strictly positive for all admissible h, such that $h(x) \equiv 0$ does not hold. That is, we find necessary and sufficient conditions for (143) to be *positive definite*.

As suggested by Gilbert A. Bliss (1925) (Sagan, 1969:396), we consider the so-called secondary variational problem

$$\begin{aligned} &\text{Minimize:} \quad A[h] = \int_a^b (Ph'^2 + Qh^2)dx, \\ &\text{with boundary conditions } h(a) = h(b) = 0. \end{aligned} \tag{146}$$

For h(x) to yield a minimum for the functional in (31), it is necessary that the first variation of the quadratic functional A *with respect to the variation h* must vanish. That is, if $\hat{h}$ is an extremum, then $\delta A[\hat{h};k] = 0$ for all admissible values of the variation k. With this in mind, we apply Definition 1 to (143) to find the first variation of A

$$\delta A[h;k] = \lim_{a \to 0} \frac{d}{d\alpha} \int_a^b \left[P(h' + \alpha k')^2 + Q(h + \alpha h)^2\right]dx = Ph'k\Big|_a^b + \int_a^b \left[-\frac{d}{dx}(Ph') + Qh\right]kdx.$$

Since the boundary conditions on h are homogeneous, then so are the boundary conditions on admissible k, and a necessary condition for $\delta A[\hat{h};k]$ to vanish for all admissible k is that the second order differential equation,

$$-\frac{d}{dx}(Ph') + Qh = 0 \tag{147}$$

must hold for all $x \in [a, b]$. Equation (147) along with the boundary conditions in (146) are satisfied by the function $h(x) \equiv 0$. This trivial solution may not be the only

solution. To develop a test for uniqueness, we begin with the definition of a conjugate point.

Definition 4. The point $\tilde{a}$ is said to be *conjugate to the point a* if the equation (147) has a solution which vanishes for x = a and x = $\tilde{a}$ buy is <u>not</u> identically zero (Gelfand & Fomin, 1963:106).

This statement of the definition of a conjugate point and the strengthened inequality in (145) lead to the next theorem.

Theorem 8. The quadratic functional

$$\int_a^b (Ph'^2 + Qh^2)dx,$$

where

$$P(x) > 0 \qquad (a \le x \le b),$$

is positive definite for all h(x) such that h(a) = h(b) = 0 if and only if the interval [a, b] contains no point conjugate to a (Gelfand & Fomin, 1963:111).

The theory that led to the definition of a conjugate point drives the analysis presented in the next section, while Theorem 8 serves as the impetus of a positive definiteness theorem for the second variation presented in the subsequent section. Finally, Section 6.4 ties together this entire document into a theorem which states sufficient conditions for the existence of a minimal solution for the optimization problem we have been examining.

6.2 *The Secondary Variational Problem and Conjugate Times*

Motivated by the theory presented in the previous section, we now examine the secondary variational problem for the quadratic functional in (126), restated as

$$A[h,\Delta\mathbf{t},\delta\mathbf{c}]=\int_0^{t_f}\left(P(t)h_t^2+R(t)h^2\right)dt+\sum_{i=1}^{n-1}[\Delta t_i \quad \delta c_i]\cdot\mathbf{M}^{(i)}\cdot\begin{bmatrix}\Delta t_i\\ \delta c_i\end{bmatrix}, \tag{148}$$

where P(t), R(t), and $\mathbf{M}^{(i)}$ are defined by (125) and the vectors $\Delta\mathbf{t}$ and $\delta\mathbf{c}$ have elements Δt_i and δc_i, respectively for i = 1, 2, ... n-1. Here, we treat the second variation of the Lagrangian as a function of its variations and seek to find conditions that assure A is a positive definite quadratic functional, thereby providing sufficient conditions to verify our solution is minimal. We start by considering admissible variations h such that $h \equiv 0$ for $t \in [0, t_{i-1}] \cup [t_{i+1}, t_f]$ which implies $\Delta t_j = \delta c_j = 0$ for all $j \neq i$ (Figure 9), so that (148) can be written as

$$A[h,\Delta t_i,\delta c_i]=\int_{t_{i-1}}^{t_{i+1}}\left(P(t)h_t^2+R(t)h^2\right)dt+[\Delta t_i \quad \delta c_i]\cdot\mathbf{M}^{(i)}\cdot\begin{bmatrix}\Delta t_i\\ \delta c_i\end{bmatrix}. \tag{149}$$

As in the case of the simplest variational problem, we now state the secondary variational problem as

$$\begin{aligned}&\text{Minimize:} \quad A[h, \Delta t_i, \delta c_i],\\ &\text{such that } h(t_{i-1}) = h(t_{i+1}) = 0\end{aligned} \tag{150}$$

for all i = 1, 2, ... n-1. The variational problem in (150) suggests that the solution $(\hat{h},\Delta\hat{t}_i,\delta\hat{c}_i)$ yields a minimum of A if the variation of A at $(\hat{h},\Delta\hat{t}_i,\delta\hat{c}_i)$, denoted as

$$\delta A = \delta A\left[\hat{h}, \Delta\hat{t}_i, \delta\hat{c}_i; k, \delta(\Delta t_i), \delta(\delta c_i)\right], \tag{151}$$

vanishes for all admissible variations $(k,\delta(\Delta t_i),\delta(\delta c_i))$. In analyzing the variational problem in (150), we arrive at a definition for *conjugate times* that is similar to Definition 4 of the previous section.

We begin the analysis by first determining the variation of A at $(h,\Delta t_i,\delta c_i)$. Without loss of generality, assume $\Delta t_i > 0$, then

$$\delta A = \lim_{a\to 0}\frac{\partial}{\partial a}\left\{\begin{array}{l}\int_{t_{i-1}}^{t_{i+1}}\left[P\left(h_t + ak_t\right)^2 + R(h+ak)^2\right]dt \\ +\left[\Delta t_i + a\delta\left(\Delta t_i\right) \quad \delta c_i + a\delta\left(\delta c_i\right)\right]\cdot \mathbf{M}^{(i)}\cdot\begin{bmatrix}\Delta t_i + a\delta\left(\Delta t_i\right)\\ \delta c_i + a\delta\left(\delta c_i\right)\end{bmatrix}\end{array}\right\}, \tag{152}$$

where the interval of integration can be written as

$$[t_{i-1}, t_{i+1}] = [t_{i-1}, t_i] \cup [t_i, t_i+\Delta t_i+a\delta(\Delta t_i)] \cup [t_i+\Delta t_i+a\delta(\Delta t_i), t_{i+1}].$$

Using Leibnitz's rule and taking the limit in (152), we have

$$\delta A = 2\int_{t_{i-1}}^{t_{i+1}}\left[Ph_t k_t + Rhk\right]dt + \left(Ph_t^2 + Rh^2\right)\Big|_{t_i+\Delta t_i+0}^{t_i+\Delta t_i-0}\delta\left(\Delta t_i\right) + 2\left[\Delta t_i \quad \delta c_i\right]\cdot \mathbf{M}^{(i)}\cdot\begin{bmatrix}\delta\left(\Delta t_i\right)\\ \delta\left(\delta c_i\right)\end{bmatrix}. \tag{153}$$

Notice that the superscripts on the second term of the right-hand side of (153) have been suppressed for notational convenience, and it should be understood that P and R are on the (i+1) interval since $\Delta t_i > 0$ was assumed. Because of the boundary conditions in (150), we assume $k(t_{i-1}) = k(t_{i+1}) = 0$, thus integrating (153) by parts yields

$$\delta A = 2\int_{t_{i-1}}^{t_{i+1}}\left[-\frac{\partial}{\partial t}(Ph_t) + Rh\right]k\,dt + \left(Ph_t^2 + Rh^2\right)\Big|_{t_i+\Delta t_i+0}^{t_i+\Delta t_i-0}\delta(\Delta t_i)$$
$$+2[\Delta t_i \quad \delta c_i]\cdot \mathbf{M}^{(i)}\cdot\begin{bmatrix}\delta(\Delta t_i)\\ \delta(\delta c_i)\end{bmatrix}. \tag{154}$$

Now, assume $(\hat{h}, \Delta\hat{t}_i, \delta\hat{c}_i)$ minimizes A. Then setting $\delta A = 0$ for all admissible variations $(k,\delta(\Delta t_i),\delta(\delta c_i))$ leads to three special cases.

Case 1. Assume $\delta(\Delta t_i) = \delta(\delta c_i) = 0$. Using the same procedure as that used in Chapters IV and V, we have the following subcases from setting $\delta A[\hat{h}, \Delta\hat{t}_i, \delta\hat{c}_i; k,0,0] = 0$:

(1a) $k = 0\ \ \forall t \in [t_i, t_{i+1}]$ implies $-\frac{\partial}{\partial t}(P\hat{h}_t) + R\hat{h} = 0\ \ \forall t \in [t_{i-1}, t_i)$.

(1b) $k = 0\ \ \forall t \in [t_{i-1}, t_i] \cup [t_i+\Delta t_i, t_{i+1}]$ implies $-\frac{\partial}{\partial t}(P\hat{h}_t) + R\hat{h} = 0\ \ \forall t \in (t_i, t_i+\Delta t_i)$.

(1c) $k = 0\ \ \forall t \in [t_{i-1}, t_i+\Delta t_i]$ implies $-\frac{\partial}{\partial t}(P\hat{h}_t) + R\hat{h} = 0\ \ \forall t \in (t_i+\Delta t_i, t_{i+1}]$.

The necessary conditions provided by case (1) reduce the first variation of A (considering the set $(\hat{h}, \Delta\hat{t}_i, \delta\hat{c}_i)$ is optimal) in (154) to

$$\delta A[\hat{h}, \Delta\hat{t}_i, \delta\hat{c}_i; k, \delta(\Delta t_i), \delta(\delta c_i)] = \left(P\hat{h}_t^2 + R\hat{h}^2\right)\Big|_{t_i+\Delta\hat{t}_i+0}^{t_i+\Delta\hat{t}_i-0}\delta(\Delta t_i) + 2[\Delta\hat{t}_i \quad \delta\hat{c}_i]\cdot\mathbf{M}^{(i)}\cdot\begin{bmatrix}\delta(\Delta t_i)\\ \delta(\delta c_i)\end{bmatrix}. \tag{155}$$

Case 2. Now, assume $\delta(\delta c_i) = 0$ and $\delta(\Delta t_i) \neq 0$, then setting(155) to zero, we have

$$\delta A[\hat{h}, \Delta\hat{t}_i, \delta\hat{c}_i; k, \delta(\Delta t_i), 0] = \left[\left(P\hat{h}_t^2 + R\hat{h}^2\right)\Big|_{t_i+\Delta\hat{t}_i+0}^{t_i+\Delta\hat{t}_i-0} + 2m_{11}\Delta\hat{t}_i + 2m_{12}\delta\hat{c}_i\right]\cdot\delta(\Delta t_i) = 0. \tag{156}$$

Since $\delta(\Delta t_i) \neq 0$, then we have the necessary condition

$$m_{11}\Delta\hat{t}_i + m_{12}\delta\hat{c}_i = -\frac{1}{2}\left(P\hat{h}_t^2 + R\hat{h}^2\right)\Big|_{t_i+\Delta\hat{t}_i+0}^{t_i+\Delta\hat{t}_i-0}, \tag{157}$$

reducing (155) to

$$\delta A\left[\hat{h},\Delta\hat{t}_i,\delta\hat{c}_i\right] = 2\left[m_{21}\Delta\hat{t}_i + m_{22}\delta\hat{c}_i\right]\cdot\delta(\delta c_i) = 0 \tag{158}$$

which leads to the final case.

<u>**Case 3**</u>. Finally, assume $\delta(\delta c_i) \neq 0$, then (158) produces the necessary condition

$$m_{21}\Delta\hat{t}_i + m_{22}\delta\hat{c}_i = 0. \tag{159}$$

Combining all three cases, we have the following necessary conditions for any optimal solution $\left(\hat{h},\Delta\hat{t}_i,\delta\hat{c}_i\right)$

$$-\frac{\partial}{\partial t}\left(P\hat{h}_t\right) + R\hat{h} = 0 \qquad \forall t \in \left(t_{i-1},t_{i+1}\right) - \left\{t_i + \Delta t_i, t_i\right\}, \tag{160}$$

and

$$\mathbf{M}^{(i)}\cdot\begin{bmatrix}\Delta\hat{t}_i\\ \delta\hat{c}_i\end{bmatrix} = -\frac{1}{2}\begin{bmatrix}\left(P\hat{h}_t^2 + R\hat{h}^2\right)\Big|_{t_i+\Delta\hat{t}_i+0}^{t_i+\Delta\hat{t}_i-0}\\ 0\end{bmatrix}. \tag{161}$$

Also, since i was chosen arbitrarily, then (160) and (161) hold for any i = 1, 2, ... n-1.

The necessary conditions in (160) and (161) resulted from an examination of the secondary variational problem. Recall, in the previous section, the similar analysis led to a definition of a conjugate point. We now state an analogous definition for the present problem.

Definition 5. (Conjugate time) The time $\hat{t} \in (a, b]$ is said to be *conjugate* to a if there exist numbers $c \in \mathbf{R}$ and $\Delta \in (0, b\text{-}c)$, and a function u(t) where

$$u(t) = \begin{cases} u^{(1)}(t) & a < t < c \\ u^{(2)}(t) & c < t < c+\Delta, \\ u^{(3)}(t) & c+\Delta < t < b \end{cases}$$

such that u(t) satisfies the boundary value problem

$$-\frac{\partial}{\partial t}\left(P^{(1)}u_t^{(1)}\right) + R^{(1)}u^{(1)} = 0 \qquad a < t < c,$$

$$-\frac{\partial}{\partial t}\left(P^{(2)}u_t^{(2)}\right) + R^{(2)}u^{(2)} = 0 \qquad c < t < c+\Delta,$$

$$-\frac{\partial}{\partial t}\left(P^{(2)}u_t^{(3)}\right) + R^{(2)}u^{(3)} = 0 \qquad c+\Delta < t < b,$$

where

$$P(t) = \begin{cases} P^{(1)}(t) & a < t < c \\ P^{(2)}(t) & c < t < b \end{cases}, \qquad \text{and} \qquad R(t) = \begin{cases} R^{(1)}(t) & a < t < c \\ R^{(2)}(t) & c < t < b \end{cases}$$

and such that

$$P^{(1)}u_t^{(1)}\Big|_{t=c} = P^{(2)}u_t^{(2)}\Big|_{t=c}, \quad u^{(1)}\Big|_{t=c} = u^{(2)}\Big|_{t=c}, \quad \text{and} \quad u^{(2)}\Big|_{t=c+\Delta} = u^{(3)}\Big|_{t=c+\Delta}.$$

Additionally,

$$\mathbf{M}^{(i)} \cdot \begin{bmatrix} \Delta t_i \\ \delta c_i \end{bmatrix} = -\frac{1}{2}\begin{bmatrix} \left(P^{(2)}\left(u_t^{(2)}\right)^2 + R^{(2)}\left(u^{(2)}\right)^2\right)\Big|_{t=c+\Delta} - \left(P^{(2)}\left(u_t^{(3)}\right)^2 + R^{(2)}\left(u^{(3)}\right)^2\right)\Big|_{t=c+\Delta} \\ 0 \end{bmatrix},$$

where $\mathbf{M}^{(i)}$ is a constant matrix whose coefficients are determined by (125) for any choice of i, and P(t) and R(t) are also as stated in (125); such that u(a) = 0 and $u(\hat{t}) = 0$ but u(t) is not identically zero (Figure 10).

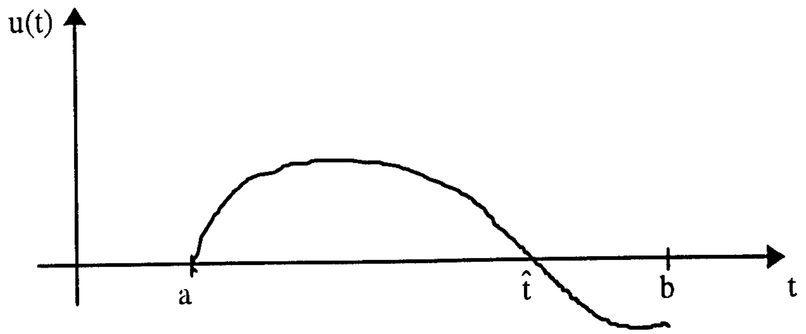

Figure 10. The time $\hat{t}$ is conjugate to the time a (Definition 5).

With the statement of this definition, the next section presents a theorem which establishes necessary and sufficient conditions for the quadratic functional in (126) to be positive definite.

6.3 *Positive Definiteness of the Second Variation of the Lagrangian*

This section establishes the positive definiteness of the second variation through the following theorem (note that P, R and $\mathbf{M}^{(i)}$ are defined by (125)).

Theorem 9. The quadratic functional

$$A[h, \Delta t_i, \delta c_i] = \int_{t_{i-1}}^{t_{i+1}} \left(P(t) h_t^2 + R(t) h^2\right) dt + \overline{\Delta}_i^T \cdot \mathbf{M}^{(i)} \cdot \overline{\Delta}_i, \tag{162}$$

where $\overline{\Delta}_i^T = \begin{bmatrix} \Delta t_i & \delta c_i \end{bmatrix}$,

$$P(t) = \begin{cases} P^{(i)}(t) & t_{i-1} < t < t_i \\ P^{(i+1)}(t) & t_i < t < t_{i+1} \end{cases}, \quad \text{and} \quad R(t) = \begin{cases} R^{(i)}(t) & t_{i-1} < t < t_i \\ R^{(i+1)}(t) & t_i < t < t_{i+1} \end{cases},$$

such that $P(t) > 0$ for all $t \in (t_{i-1}, t_i) \cup (t_i, t_{i+1})$, and $\mathbf{M}^{(i)}$ is a nonnegative definite matrix (denoted by $\mathbf{M}^{(i)} \geq 0$), is a positive definite functional for all h(t) such that $h(t_{i-1}) = 0$ and $h(t_{i+1}) = 0$ if and only if the interval $[t_{i-1}, t_{i+1}]$ contains no conjugate times to t_{i-1}.

Proof. ($\Leftarrow$) The fact that the functional in (162) is positive definite will be proved if we can reduce it to the form

$$\int_{t_{i-1}}^{t_{i+1}} P(t)\varphi^2 dt + \overline{\Delta}_i^T \cdot \tilde{\mathbf{M}}^{(i)} \cdot \overline{\Delta}_i,$$

where φ^2 is some function which cannot be identically zero unless $h(t) \equiv 0$ and $\tilde{\mathbf{M}}^{(i)} \geq 0$. To achieve this goal, we add a quantity of the form $\frac{d}{dt}(wh^2)$ to the integrand of (162), where w(t) is a differentiable function, which is continuous at t_i. Notice, because of the corner at t_i and since $h(t_{i-1}) = h(t_{i+1}) = 0$, then

$$\int_{t_{i-1}}^{t_{i+1}} \frac{d}{dt}(wh^2)dt - \left(wh^2\right)\Big|_{t_i+0}^{t_i-0} = 0,$$

where $h(t_i) = h(\mathbf{x}_w,t_i) = \delta c_i - c_t(\mathbf{x}_w,t_i)\Delta t_i$. Now, choose w(t) such that

$$Ph_t^2 + Rh^2 + \frac{d}{dt}(wh^2) = Ph_t^2 + 2whh_t + \left(R + w_t\right)h^2 \tag{163}$$

is a perfect square and the expression

$$\overline{\Delta}_i^T \cdot \mathbf{M}^{(i)} \cdot \overline{\Delta}_i - \left[w\left(\delta c_i - c_t \Delta t_i\right)^2\right]\Big|_{t_i+0}^{t_i-0} \tag{164}$$

is nonnegative for any $\overline{\Delta}_i$.

Notice, the second term in (164) can be written as

$$\left[w\left(\delta c_i - c_t \Delta t_i\right)^2\right]\Big|_{t_i+0}^{t_i-0} = w\left(\delta c_i^2 - 2c_t \delta c_i \Delta t_i + c_t^2 \Delta t_i^2\right)\Big|_{t_i+0}^{t_i-0}$$

$$= \overline{\Delta}_i^T \cdot \begin{bmatrix} w\Big|_{t_i+0}^{t_i-0} & -wc_t\Big|_{t_i+0}^{t_i-0} \\ -wc_t\Big|_{t_i+0}^{t_i-0} & wc_t^2\Big|_{t_i+0}^{t_i-0} \end{bmatrix} \cdot \overline{\Delta}_i,$$

and since w(t) is continuous at t_i, then (164) can be written as

$$\overline{\Delta}_i^T \cdot \mathbf{M}^{(i)} \cdot \overline{\Delta}_i - \left[w\left(\delta c_i - c_t \Delta t_i\right)^2\right]\Big|_{t_i+0}^{t_i-0} = \overline{\Delta}_i^T \cdot \begin{bmatrix} m_{11} & m_{12} + wc_t\Big|_{t_i+0}^{t_i-0} \\ m_{12} + wc_t\Big|_{t_i+0}^{t_i-0} & m_{22} - wc_t^2\Big|_{t_i+0}^{t_i-0} \end{bmatrix} \cdot \overline{\Delta}_i$$

$$= \overline{\Delta}_i^T \cdot \tilde{\mathbf{M}}^{(i)} \cdot \overline{\Delta}_i .$$

According to a well known result, sometimes called *Sylvester's criterion*, a 2 x 2 matrix **A** is nonnegative definite if and only if the descending principal minors

$$a_{11} \qquad \text{and} \qquad \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}$$

of the matrix are both nonnegative. For the matrix $\tilde{\mathbf{M}}^{(i)}$ above, we know that the term $a_{11} = m_{11}$ is necessarily nonnegative by (138). Thus, if $\det\tilde{\mathbf{M}}^{(i)}$ is nonnegative, then the matrix $\tilde{\mathbf{M}}^{(i)}$ is nonnegative. Therefore, computing the determinant

$$\det\tilde{\mathbf{M}}^{(i)} = m_{11}\left(m_{22} - wc_t^2\Big|_{t_i+0}^{t_i-0}\right) - \left(m_{12} + wc_t\Big|_{t_i+0}^{t_i-0}\right)^2$$

$$= \underbrace{m_{11}m_{22} - m_{12}^2}_{\det\mathbf{M}^{(i)}=\gamma} - \underbrace{\left[m_{11}\left(c_t^2\right)\Big|_{t_i+0}^{t_i-0} + 2m_{12}\left(c_t\Big|_{t_i+0}^{t_i-0}\right)\right]}_{\beta} w(t_i) \underbrace{-\left(c_t\Big|_{t_i+0}^{t_i-0}\right)^2}_{\alpha}\left[w(t_i)\right]^2,$$

where $w(t_i)$ has been factored out since w is continuous at t_i. Thus, we can write

$$\det\tilde{\mathbf{M}}^{(i)} = \alpha\left[w(t_i)\right]^2 + \beta w(t_i) + \gamma, \tag{165}$$

where $\alpha \leq 0$, $\gamma \geq 0$, and β could be positive, negative or zero, and we will assume it is not zero. We see that (165) is quadratic in w for any fixed i. If the quadratic (165) has two real zeroes, then there exists w such that $\det\tilde{\mathbf{M}}^{(i)} \geq 0$, implying that $\tilde{\mathbf{M}}^{(i)} \geq 0$. This will be the case if

$$\beta^2 - 4\alpha\gamma = \beta^2 - 4\left[-\left(c_t\Big|_{t_i+0}^{t_i-0}\right)^2 \det\mathbf{M}^{(i)}\right] = \beta^2 + 4\left[\left(c_t\Big|_{t_i+0}^{t_i-0}\right)^2 \det\mathbf{M}^{(i)}\right] > 0,$$

which is true, as long as $\beta \neq 0$. Thus, (165) has two real roots for any choice of i which implies w(t) exists such that $\tilde{\mathbf{M}}^{(i)} \geq 0$.

Let $W = \{w \mid w \text{ is continuous at } t_i \text{ and } \tilde{\mathbf{M}}^{(i)} \geq 0\}$ and choose $w \in W$ such that

$$P(R + w_t) = w^2. \tag{166}$$

If (166) holds on the entire interval $[t_{i-1}, t_{i+1}]$, then the quadratic functional (162) can be written as

$$\int_{t_{i-1}}^{t_{i+1}} P\left(h_t + \frac{w}{P}h\right)^2 dt + \bar{\Delta}_i^T \cdot \tilde{\mathbf{M}}^{(i)} \cdot \bar{\Delta}_i, \tag{167}$$

and is therefore nonnegative. Since $P > 0$, then (167) will vanish only if the following <u>both</u> occur simultaneously:

$$\begin{aligned} &h_t + \frac{w}{P}h \equiv 0 && t \in [t_{i-1}, t_{i+1}] - \{t_i, t_i + \Delta t_i\} \\ \text{and} \\ &\bar{\Delta}_i^T \tilde{\mathbf{M}}^{(i)} \bar{\Delta}_i \equiv 0 && t_i \in [t_{i-1}, t_{i+1}]. \end{aligned} \tag{168}$$

The boundary condition $h(t_{i-1}) = 0$ implies $h(t) \equiv 0$. Since $h \equiv 0$ for all t, then $\Delta t_i = \delta c_i = 0$ and $\bar{\Delta}_i^T \tilde{\mathbf{M}}^{(i)} \bar{\Delta}_i \equiv 0$. So, both conditions in (168) occur only if $h(t) \equiv 0$, and it follows that (167) is actually positive definite.

Now, the proof has been reduced to showing that the absence of times in $[t_{i-1}, t_{i+1}]$ which are conjugate to t_{i-1} guarantees (166) has a solution defined on the whole interval. First, we introduce the change of variables

$$w = -\frac{u_t}{u}P, \qquad \text{where } u(t) = \begin{cases} u^{(1)}(t) & t_{i-1} < t < t_i \\ u^{(2)}(t) & t_i < t < t_i + \Delta t_i \\ u^{(3)}(t) & t_i + \Delta t_i < t < t_{i+1} \end{cases}$$

into (166), where u is a new unknown function such that

$$P^{(i)}u_t^{(1)}\Big|_{t=t_i} = P^{(i+1)}u_t^{(2)}\Big|_{t=t_i}, \qquad u^{(1)}\Big|_{t=t_i} = u^{(2)}\Big|_{t=t_i}, \quad \text{and} \quad u^{(2)}\Big|_{t=t_i+\Delta t_i} = u^{(3)}\Big|_{t=t_i+\Delta t_i},$$

then equation (166) becomes

$$
\begin{aligned}
&-\frac{\partial}{\partial t}\left(P^{(i)}u_t^{(1)}\right) + R^{(i)}u^{(1)} = 0 && t_{i-1} < t < t_i, \\
&-\frac{\partial}{\partial t}\left(P^{(i+1)}u_t^{(2)}\right) + R^{(i+1)}u^{(2)} = 0 && t_i < t < t_i + \Delta t_i, \\
&-\frac{\partial}{\partial t}\left(P^{(i+1)}u_t^{(3)}\right) + R^{(i+1)}u^{(3)} = 0 && t_i + \Delta t_i < t < t_{i+1}.
\end{aligned}
\tag{169}
$$

If there are no times conjugate to t_{i-1} in $(t_{i-1}, t_{i+1}]$ then (169) has a solution which does not vanish anywhere in $(t_{i-1}, t_{i+1}]$. Since the solution to the differential equation in (169) depends continuously on the initial conditions, then $[t_{i-1}, t_{i+1}]$ contains no times which are conjugate to $t_{i-1} - \varepsilon$ for some sufficiently small ε (Sagan, 1969:402). Therefore, a solution exists for (169) which does not vanish anywhere in $[t_{i-1}, t_{i+1}]$ which implies (166) is valid throughout the entire interval and in turn, (162) is positive definite.

($\Rightarrow$) Suppose now that $t_{i-1} < \hat{t} < t_{i+1}$, that is, the interval (t_{i-1}, t_{i+1}) contains at least one time which is conjugate to t_{i-1}, which implies there exists a nontrivial solution $h = h^*(x)$ of equation (169) such that

$$h^*(t_{i-1}) = h^*(\hat{t}) = 0, \quad \text{but } h^*(t) \neq 0 \text{ for } t \in (t_{i-1}, \hat{t}).$$

Since $h = h(t) \equiv 0$ is also a solution of (169), then the function

$$h = \bar{h}(t) \equiv \begin{cases} h^*(t) & \text{for } t_{i-1} \leq t \leq \hat{t} \\ 0 & \text{for } \hat{t} \leq t \leq t_{i+1} \end{cases} \tag{170}$$

is a sectionally smooth solution of equation (169) (Figure 11). Choose $\hat{t} < t_i$ then the quadratic functional given by (162) becomes

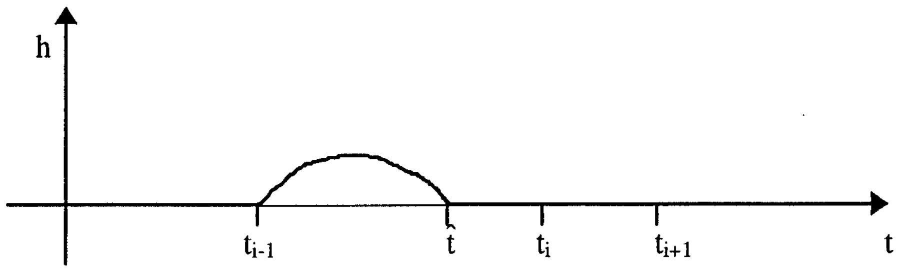

Figure 11. A nontrivial solution h for equation (169).

$$A[\bar{h}, \Delta t_i = 0, \delta c_i = 0] = \int_{t_{i-1}}^{\hat{t}} \left[P(h^*)_t^2 + R(h^*)^2\right] dt,$$

since $h(t_i) \equiv 0$ implies $\Delta t_i = \delta c_i = 0$. Integrating the above expression by parts, we have

$$A[\bar{h}, \Delta t_i = 0, \delta c_i = 0] = Ph^*(h^*)_t \Big|_{t_{i-1}}^{\hat{t}} + \int_{t_{i-1}}^{\hat{t}} h^* \left[-\frac{\partial}{\partial t}\left(P(h^*)_t\right) + Rh^*\right] dt = 0,$$

since we know that $h^*(t_{i-1}) = h^*(\hat{t}) = 0$ and $h^*(t)$ satisfies (169). Thus we have shown that $A[\bar{h}, \Delta t_i = 0, \delta c_i = 0] = 0$. Suppose that 0 is the minimum of $A[h, \Delta t_i, \delta c_i]$, then it is necessary that $h = \bar{h}(t)$, which produced the minimum value 0, must satisfy the corner condition at $t = \hat{t}$ (equation (83), for example)

$$g_{h_t}\Big|_{\hat{t}-0} = g_{h_t}\Big|_{\hat{t}+0},$$

where $g = Ph_t^2 + Rh^2$. Since $g_{h_t} = 2Ph_t$, then for $h = \bar{h}(t)$ we have

$$g_{h_t}\Big|_{\hat{t}-0} = 2P(\hat{t})(h^*)_t(\hat{t})$$

and (171)

$$g_{h_t}\Big|_{\hat{t}+0} = 0.$$

By hypothesis, we have assumed $P(t) > 0$ holds for all $t \in [t_{i-1}, t_{i+1}]$ and thus, the corner condition (171) can only be satisfied if $(h^*)_t(\hat{t} - 0) = 0$. Since we also know that

$h^*(\hat{t}) = 0$ then it follows that $h^*(t) = 0$ for all $t \in [t_{i-1}, \hat{t}]$, violating the assumption that we have a nontrivial solution, $h = h^*(t)$, for equation (169).

Since $h = \bar{h}(t)$ defined by (170) does not satisfy the necessary condition for a minimum stated in (171), then $A[\bar{h}, \Delta t_i = 0, \delta c_i = 0] = 0$ cannot be the minimum of the quadratic functional A. Hence there exists a function $h = \bar{\bar{h}}(t)$ with a corner at $t = \hat{t}$ such that $A[\bar{\bar{h}}, \Delta t_i = 0, \delta c_i = 0] < 0$. Then, by a well known result sometimes referred to as the fairing theorem [Sagan, 1969], there exists a function $h \in C^1[t_{i-1}, t_{i+1}]$, $h(t_{i-1}) = h(t_{i+1}) = 0$, such that $A[h, \Delta t_i, \delta c_i] < 0$. Thus, we have proven that the existence of conjugate times to t_{i-1} in the interval $(t_{i-1}, t_{i+1}]$ implies that A is <u>not</u> positive definite. By the contrapositive proof form, this is true if and only if A is positive definite implies that the interval contains no conjugate times. $\square$

With the proof of Theorem 9, we have all the pieces needed to state the sufficient conditions for the existence of a minimum solution for the optimization problem of Chapter III. Thus far, we have established necessary conditions for a minimum all of which could be considered separately, since each is necessary by itself. The sufficient conditions stated in the next section, which are similar to the necessary conditions, must be considered as a set since a minimal solution is only guaranteed if all the conditions are satisfied simultaneously.

6.4 *Sufficient Conditions for a Minimum*

This section presents a set of conditions in the form of a theorem which, if met by any admissible functions (Q, c, λ), then the Lagrangian given in equation (39) is guaranteed to have a minimum for the given solution. Again, these sufficient conditions are presented as a set, and the presence of an extremal is only assured if all the conditions are satisfied.

Before examining this theorem, we must define a norm for the space in which we are working. Notice, if the functions ($\hat{Q}$, $\hat{c}$, $\hat{\lambda}$) minimize the Lagrangian in (39) then the increment of $\mathcal{L}$, defined as

$$\Delta\mathcal{L} = \mathcal{L}(\hat{Q} + K, \hat{c} + h, \hat{\lambda} + \mu) - \mathcal{L}(\hat{Q}, \hat{c}, \hat{\lambda}), \tag{172}$$

must be nonnegative, where $(\hat{Q} + K, \hat{c} + h, \hat{\lambda} + \mu)$ are functions sufficiently close to the functions ($\hat{Q}$, $\hat{c}$, $\hat{\lambda}$). In determining the closeness of these functions, we make the following definition.

Definition 6. Let S = {Q(t):[a, b] $\rightarrow$ {0, Q_{ON}}, such that Q(t) is piecewise constant}. Given that Q $\in$ S, c $\in$ C^1[a, b], and $\lambda \in$ C[a, b] define the norm $\|*\|_{\bar{1}}$ by

$$\|(Q, c, \lambda)\|_{\bar{1}} = \|Q\|_{L_1} + \|c\|_1 + \|\lambda\|_0,$$

such that

$$\|Q\|_{L_1} = \int_a^b |Q| dt, \qquad \|c\|_1 = \max_{a \le t \le b} |c(t)| + \max_{a \le t \le b} |c_t(t)|, \quad \text{and} \qquad \|\lambda\|_0 = \max_{a \le t \le b} |\lambda(t)|.$$

Note that two functions $(\hat{Q}, \hat{c}, \hat{\lambda})$ and (Q, c, λ), defined on the interval [a, b] as stated in Definition 6 are regarded as close together if

$$\left\|(\hat{Q},\hat{c},\hat{\lambda}) - (Q,c,\lambda)\right\|_{\bar{I}} < \varepsilon$$

for all $\varepsilon > 0$.

Theorem 10. Suppose that for some admissible functions $(\hat{Q}, \hat{c}, \hat{\lambda})$ the Lagrangian (39) for the optimization problem defined by (24) - (27) satisfies the following conditions:

1. The functions $(\hat{Q}, \hat{c}, \hat{\lambda})$ are an extremal, and hence the first variation of (39) vanishes; implying that the conditions stated in (75), (78), (81), (83), (84), (89), (91), and (95) are met.

2. For the functions $(\hat{Q}, \hat{c}, \hat{\lambda})$,

$$P^{(i)}(t) \equiv \frac{1}{2} f_{c_t c_t}[t, \hat{Q}^{(i)}(t), \hat{c}^{(i)}(\mathbf{x}_w t), \hat{c}_t^{(i)}(\mathbf{x}_w t)] > 0 \tag{173}$$

for all $t \in [t_{i-1}, t_i]$, and for all i = 1, 2, ... n, and

$$\mathbf{M}^{(i)} \geq 0 \tag{174}$$

for all i = 1, 2, ... n-1, where $\mathbf{M}^{(i)}$ is given as

$$\mathbf{M}^{(i)} = \frac{1}{2}\begin{bmatrix} \left(\hat{f}_t - \hat{f}_c \hat{c}_t - \hat{f}_{c_t} \hat{c}_{tt} + \hat{f}_{cc_t} \hat{c}_t^2\right)\Big|_{t_i+0}^{t_i-0} & \left(\hat{f}_c - \hat{f}_{cc_t} \hat{c}_t\right)\Big|_{t_i+0}^{t_i-0} \\ \left(\hat{f}_c - \hat{f}_{cc_t} \hat{c}_t\right)\Big|_{t_i+0}^{t_i-0} & \hat{f}_{cc_t}\Big|_{t_i+0}^{t_i-0} \end{bmatrix}_{\mathbf{x}=\mathbf{x}_w}$$

and

$$m_{11}^{(i)} = \frac{1}{2}\left[\hat{f}_t - \hat{f}_c \hat{c}_t - \hat{f}_{c_t} \hat{c}_{tt} + \hat{f}_{cc_t} \hat{c}_t^2\right]_{\mathbf{x}=\mathbf{x}_w}\Big|_{t_i+0}^{t_i-0} \geq 0,$$

$$m_{22}^{(i)} = \frac{1}{2}\left[\hat{f}_{cc_t}\right]_{\mathbf{x}=\mathbf{x}_w}\Big|_{t_i+0}^{t_i-0} > 0.$$

3. The time interval $[t_{i-1}, t_{i+1}]$, contains no times which are conjugate to the time t_{i-1}, for all i = 1, 2, ... n.

Then the functional in (24), constrained by the conditions in (25) - (27) has a minimum at $(\hat{Q}, \hat{c}, \hat{\lambda})$ with respect to $\|*\|_{\bar{1}}$.

Proof. The theorem is proved if we show that, for any sufficiently close (in the sense of $\|*\|_{\bar{1}}$) functions to those given as the extremal $(\hat{Q}, \hat{c}, \hat{\lambda})$, the increment in (172) is positive. Suppose the functions $(\hat{Q}, \hat{c}, \hat{\lambda})$ and $(\hat{Q}+K, \hat{c}+h, \hat{\lambda}+\mu)$ are sufficiently close. That is, given $\varepsilon > 0$, then

$$\|(K, h, \mu)\|_{\bar{1}} < \varepsilon,$$

which implies

$$\|K\|_{L_1} < \varepsilon, \qquad \|h\|_1 < \varepsilon, \quad \text{and} \qquad \|\mu\|_0 < \varepsilon.$$

Thus, we can use Taylor's theorem to find that the increment can be written as

$$\begin{aligned} \Delta\mathcal{L} &= \mathcal{L}(\hat{Q} + K, \hat{c} + h, \hat{\lambda} + \mu) - \mathcal{L}(\hat{Q}, \hat{c}, \hat{\lambda}) \\ &= \delta\mathcal{L} + \delta^2\mathcal{L} + \sigma, \end{aligned} \tag{175}$$

where σ is an infinitesimal of order higher than 2 relative to $\|(K, h, \mu)\|_{\bar{1}}^2$ (Gelfand & Fomin, 1963:101). The first term above is the first variation of the Lagrangian which vanishes according to condition 1, and the second term is the second variation of the Lagrangian, stated in (126). Alternatively, (175) can be written as

$$\Delta\mathcal{L} = \int_0^{t_f}\left(P(t)h_t^2 + R(t)h^2\right)dt + \sum_{i=1}^{n-1}\overline{\Delta}_i^T \cdot \mathbf{M}^{(i)} \cdot \overline{\Delta}_i + \int_0^{t_f}\left(\eta h_t^2 + \xi h^2\right)dt + \sum_{i=1}^{n-1}\overline{\Delta}_i^T \cdot \widetilde{\mathbf{M}}^{(i)} \cdot \overline{\Delta}_i, \quad (176)$$

where $\xi(t)$, $\eta(t)$, and $\tilde{m}_{j,k}(t_i) \to 0$ as $\|(K,h,\mu)\|_{\mathrm{I}} \to 0$ and $\tilde{m}_{j,k}(t_i)$ are the elements of the matrix $\widetilde{\mathbf{M}}^{(i)}$. Thus,

$$|\xi(t)| < \varepsilon, \qquad |\eta(t)| < \varepsilon, \text{ and } \qquad |\tilde{m}_{j,k}(t_i)| < \varepsilon.$$

for $0 \le t \le t_f$, and for all i =1, 2, ... n-1. The last two terms in (176) are the remainder terms of the Taylor series expansion of the increment of (175). Notice that

$$\|(K,h,\mu)\|_{\mathrm{I}} \to 0,$$

implies that

$$\|K\|_{L_1} \to 0, \qquad \|h\|_1 \to 0, \qquad \text{and} \qquad \|\mu\|_0 \to 0.$$

Since the Lagrangian is affine in the multiplier λ, then the higher order terms in μ vanish. Also, recall that a variation of the pumping rate, Q(t), depends on the switching times of the pump status. Thus,

$$\|K\|_{L_1} = \int_a^b \left|\hat{Q} + K - \hat{Q}\right| dt = Q_{ON}\sum_{i=1}^{n-1}|\Delta t_i|,$$

and $\|K\|_{L_1} \to 0$ implies that $|\Delta t_i| \to 0$ for all i = 1, 2, ... n-1. Finally, recall from (58) that

$$h(t_i) = \delta c_i - \hat{c}_t(t_i)\Delta t_i,$$

then $\|h\|_1 \to 0$ means that

$$\left|h(t_i)\right| = \left|\delta c_i - \hat{c}_t(t_i)\Delta t_i\right| \to 0.$$

Since $\left|h(t_i)\right| \to 0$ and $\left|\Delta t_i\right| \to 0$ for all i = 1, 2, ... n-1, then we must have $\left|\delta c_i\right| \to 0$ for all i = 1, 2, ... n-1. Combining all these facts, we can restate (176) as

$$\Delta \ell = \int_0^{t_f} \left(P(t)h_t^2 + R(t)h^2\right)dt + \sum_{i=1}^{n-1} \overline{\Delta}_i^T \cdot \mathbf{M}^{(i)} \cdot \overline{\Delta}_i + \int_0^{t_f} \left(\eta h_t^2 + \xi h^2\right)dt + \sum_{i=1}^{n-1} \overline{\Delta}_i^T \cdot \tilde{\mathbf{M}}^{(i)} \cdot \overline{\Delta}_i, \quad (177)$$

where $\xi(t)$, $\eta(t)$, and $\tilde{m}_{j,k}(t_i) \to 0$ as $\|h\|_1 \to 0$, $\left|\Delta t_i\right| \to 0$, and $\left|\delta c_i\right| \to 0$ for all i = 1, 2, ... n-1. So, for two sufficiently close functions, the variations h, Δt_i, and δc_i are small.

Next, we examine each term in (177) to show that this expression is always positive. Consider the first two terms in (177). If the interval $[t_{i-1}, t_{i+1}]$ contains no times which are conjugate to t_{i-1}, and if $P(t) > 0$ in $[t_{i-1}, t_{i+1}]$, then we can find a larger interval $[t_{i-1}, t_{i+1} + \varepsilon]$ which also contains no times which are conjugate to t_{i-1}, such that $P(t) > 0$ in $[t_{i-1}, t_{i+1} + \varepsilon]$ [Sagan, 1969]. Consider the quadratic functional

$$\int_{t_{i-1}}^{t_{i+1}} \left(P(t)h_t^2 + R(t)h^2\right)dt - \alpha^2 \int_{t_{i-1}}^{t_{i+1}} h_t^2 dt + \overline{\Delta}_i^T \cdot \mathbf{M}^{(i)} \cdot \overline{\Delta}_i. \quad (178)$$

Since $P(t) > 0$ in $[t_{i-1}, t_{i+1} + \varepsilon]$ and hence has a positive lower bound on this interval, then for all sufficiently small α (and assuming $\Delta t_i > 0$), we have

(a) $P(t) - \alpha^2 > 0$, for all $t_{i-1} \le t \le t_{i+1}$.

(b) The solution of the differential equations

$$-\frac{\partial}{\partial t}\left[\left(P^{(i)}-\alpha^2\right)h_t^{(1)}\right]+R^{(i)}h^{(1)}=0 \qquad t_{i-1}<t<t_i,$$

$$-\frac{\partial}{\partial t}\left[\left(P^{(i+1)}-\alpha^2\right)h_t^{(2)}\right]+R^{(i+1)}h^{(2)}=0 \qquad t_i<t<t_i+\Delta t_i,$$

$$-\frac{\partial}{\partial t}\left[\left(P^{(i+1)}-\alpha^2\right)h_t^{(3)}\right]+R^{(i+1)}h^{(3)}=0 \qquad t_i+\Delta t_i<t<t_{i+1},$$

where $h^{(i)}$ is defined on the intervals above, satisfying the boundary conditions $h(t_{i-1}) = 0$, and $h_t(t_{i-1}) = 1$ does not vanish for $t_{i-1} < t \leq t_{i+1}$.

As shown by the proof of the sufficiency statement of Theorem 9, these two conditions imply that (178) is positive definite for all sufficiently small α. That is, there exists some real number $c > 0$ such that

$$\int_{t_{i-1}}^{t_{i+1}}\left(P(t)h_t^2+R(t)h^2\right)dt+\overline{\Delta}_i^T\cdot\mathbf{M}^{(i)}\cdot\overline{\Delta}_i>c\int_{t_{i-1}}^{t_{i+1}}h_t^2dt. \tag{179}$$

Since i is arbitrary then (179) is true for all $i = 1, 2, \ldots n-1$. Thus we can write

$$\int_0^{t_f}\left(P(t)h_t^2+R(t)h^2\right)dt+\sum_{i=1}^{n-1}\overline{\Delta}_i^T\cdot\mathbf{M}^{(i)}\cdot\overline{\Delta}_i>c\int_0^{t_f}h_t^2dt. \tag{180}$$

Next, using the Schwartz inequality, we find

$$h^2(t)=\left(\int_0^t h_t(\tau)d\tau\right)^2\leq\int_0^t 1^2\cdot h_t^2(\tau)d\tau=t\int_0^t h_t^2(\tau)d\tau\leq t\int_0^{t_f}h_t^2(\tau)d\tau,$$

and integrating this expression, we then have

$$\int_0^{t_f} h^2(t)dt \le \frac{t_f^2}{2}\int_0^{t_f} h_t^2(t)dt.$$

Given that $|\xi(t)| < \varepsilon$ and $|\eta(t)| < \varepsilon$, the statement above implies that

$$\left|\int_0^{t_f}\left(\eta h_t^2 + \xi h^2\right)dt\right| \le \varepsilon\left(1+\frac{t_f^2}{2}\right)\int_0^{t_f} h_t^2(t)dt. \tag{181}$$

Finally, we examine the remaining term in (177). From the triangle inequality we have

$$\begin{aligned}
\left|\sum_{i=1}^{n-1}\overline{\Delta}_i^T\cdot\widetilde{\mathbf{M}}^{(i)}\cdot\overline{\Delta}_i\right| &\le \sum_{i=1}^{n-1}\left|\overline{\Delta}_i^T\cdot\widetilde{\mathbf{M}}^{(i)}\cdot\overline{\Delta}_i\right| \\
&= \sum_{i=1}^{n-1}\left|\tilde{m}_{11}^{(i)}\Delta t_i^2 + 2\tilde{m}_{12}^{(i)}\Delta t_i\delta c_i + \tilde{m}_{22}^{(i)}\delta c_i^2\right| \\
&\le \sum_{i=1}^{n-1}\left|\tilde{m}_{11}^{(i)}\right|\Delta t_i^2 + 2\left|\tilde{m}_{12}^{(i)}\right|\cdot\left|\Delta t_i\right|\cdot\left|\delta c_i\right| + \left|\tilde{m}_{22}^{(i)}\right|\delta c_i^2 \\
&\le \sum_{i=1}^{n-1}\max_{\substack{j=1,2\\k=1,2}}\left|\tilde{m}_{j,k}^{(i)}\right|\cdot\left(\Delta t_i^2 + 2\left|\Delta t_i\right|\cdot\left|\delta c_i\right| + \delta c_i^2\right) \\
&\le \varepsilon\sum_{i=1}^{n-1}\left(\Delta t_i^2 + 2\left|\Delta t_i\right|\cdot\left|\delta c_i\right| + \delta c_i^2\right).
\end{aligned} \tag{182}$$

Combining the inequalities of (180), (181), and (182), we have

$$\begin{aligned}
&\int_0^{t_f}\left(P(t)h_t^2 + R(t)h^2\right)dt + \sum_{i=1}^{n-1}\overline{\Delta}_i^T\cdot\mathbf{M}^{(i)}\cdot\overline{\Delta}_i + \int_0^{t_f}\left(\eta h_t^2 + \xi h^2\right)dt + \sum_{i=1}^{n-1}\overline{\Delta}_i^T\cdot\widetilde{\mathbf{M}}^{(i)}\cdot\overline{\Delta}_i \\
&\qquad > c\int_0^{t_f} h_t^2 dt - \varepsilon\left(1+\frac{t_f^2}{2}\right)\int_0^{t_f} h_t^2(t)dt - \varepsilon\sum_{i=1}^{n-1}\left(\Delta t_i^2 + 2\left|\Delta t_i\right|\cdot\left|\delta c_i\right| + \delta c_i^2\right).
\end{aligned}$$

Since $\varepsilon > 0$ can be chosen to be arbitrarily small, the expression above will be positive for all sufficiently small $\|(K,h,\mu)\|_{\mathrm{T}}$, and the extremal $(\hat{Q},\ \hat{c},\ \hat{\lambda})$ corresponds to a minimum of

the optimization problem of Chapter III. This proves the theorem, and establishes sufficient conditions for the existence of a minimum with respect to the norm $\|*\|_{I}$. □

6.5 *Summary*

Theorem 10 concludes the variational analysis of the optimization problem of Chapter III, and with it we have the desired necessary and sufficient conditions needed to establish a minimal solution. In the next chapter, we examine various combinations of the independent variables t, Q(t), c(t), and $c_t(t)$ for the functional presented in (24) to establish NOCs and SOCs for general classes of functionals. Several specific examples are also presented and discussed.

VII. General Classes of Functionals and Examples

The analysis presented thus far in this document develops a mathematical tool which can be used to derive an optimal pulsed pumping schedule at an existing pump-and -treat remediation site. This chapter investigates general classes of functionals, for which we seek to determine if an optimal pulsed pumping schedule is feasible, and then looks more closely at specific classes of interest.

The first section of this chapter examines the 15 different possibilities for different combinations of the independent variables in the argument list of the objective functional. Additionally, a comparison to Hartman's (1994) results is presented for the classes that are independent of the time derivative of the concentration. Finally, classes of interest are identified which are further studied in section 7.2, leading to specific examples which demonstrate how the complicated analysis of the previous chapters reduces to simple, usable tests.

7.1 Introduction: General Classes

In this section, we examine the 15 different possibilities for the independent variables t, Q(t), $c(\mathbf{x}_w,t)$, and $c_t(\mathbf{x}_w,t)$ contained in the argument list for the objective functional in (24). For those classes which are independent of the time derivative of the concentration, we compare to Hartman's (1994) results and draw conclusions about the feasibility of using pulsed pumping as an optimal remediation technique. Further, we

examine the additional cases provided by considering $c_t(\mathbf{x}_w,t)$ as part of the objective we wish to optimize. The section concludes by identifying specific classes of interest which will be further examined in the remainder of this chapter.

7.1.1 Comparison to Previous Results: Functionals Independent of $c_t(\mathbf{x}_w,t)$. Consider the optimization problem (presented in Chapter III) in two space dimensions where (24) is replaced by

$$J[Q,c] = \int_0^{t_f}\int_{\Gamma_1} f(t,Q(t),c(s,t))ds_1 dt, \tag{183}$$

constrained by the two-dimensional integro-differential equation, boundary conditions and initial conditions in (25), (26), and (27), respectively. For the functional in (183), we consider seven general classes of functionals to be optimized, dictated by the different combinations of the variables t, Q(t), and c(s,t); ignoring the time rate of change for the concentration as part of the objective functional. For this problem, suppose the functions $(\hat{Q},\hat{c},\hat{\lambda})$ are an extremal, then the necessary conditions which generate the candidate optimal pulsed pumping schedule (equation (95)) become

$$\begin{aligned} &f[t_i,\hat{Q}^{(i)},\hat{c}(\mathbf{x}_w,t_i)] - f[t_i,\hat{Q}^{(i+1)},\hat{c}(\mathbf{x}_w,t_i)] \\ &\quad - \hat{c}(\mathbf{x}_w,t_i)\left\{f_c[t_i,\hat{Q}^{(i)},\hat{c}(\mathbf{x}_w,t_i)] - f_c[t_i,\hat{Q}^{(i+1)},\hat{c}(\mathbf{x}_w,t_i)]\right\} = 0 \end{aligned} \tag{184}$$

for all i = 1, 2, ... n-1, where $\hat{Q}^{(i)}$ and $\hat{Q}^{(i+1)}$ are defined by equation (43) for the extremal $\hat{Q}(t)$. The roots, t_i, of equation (184) are determined strictly by information about the contaminant concentration levels observed at the extraction well. In turn, these roots

generate the switching times and establish a pulsed pumping schedule for a particular management objective.

Suppose we consider a single cycle of a piecewise constant pulsed pumping schedule (Figure 2). Then, for the switching times t_1 and t_2, equation (184) becomes

$$\begin{aligned} & f[t_1, Q_{ON}, \hat{c}(\mathbf{x}_w, t_1)] - f[t_1, 0, \hat{c}(\mathbf{x}_w, t_1)] \\ & \quad - \hat{c}(\mathbf{x}_w, t_1)\{f_c[t_1, Q_{ON}, \hat{c}(\mathbf{x}_w, t_1)] - f_c[t_1, 0, \hat{c}(\mathbf{x}_w, t_1)]\} = 0 \end{aligned} \tag{185}$$

and

$$\begin{aligned} & f[t_2, 0, \hat{c}(\mathbf{x}_w, t_2)] - f[t_2, Q_{ON}, \hat{c}(\mathbf{x}_w, t_2)] \\ & \quad - \hat{c}(\mathbf{x}_w, t_2)\{f_c[t_2, 0, \hat{c}(\mathbf{x}_w, t_2)] - f_c[t_2, Q_{ON}, \hat{c}(\mathbf{x}_w, t_2)]\} = 0, \end{aligned} \tag{186}$$

which are identical to equations (8) and (9), Hartman's necessary optimality conditions of the first variation for this functional on a radially symmetric aquifer. With this agreement of results, we can accept Hartman's analysis of the seven general classes determined by the various combinations of t, Q(t), and c(s,t) for the functional in (183) and his findings are summarized in Table 1 (Hartman, 1994:Ch 4). Since equations (185) and (186)

Table 1.

General Classes of Functionals Independent of $c_t(\mathbf{x}_w,t)$.

General Class	Nature of Equation (184)	Pulsed Pumping Alternative	Interesting Objectives
f(t)	identically zero	yes	no
f(Q(t))	no roots	no	no
$f(c(\mathbf{x}_w,t))$	identically zero	yes	no
f(t, Q(t))	possibly distinct roots	yes	no
$f(t,c(\mathbf{x}_w,t))$	identically zero	yes	no
$f(Q(t),c(\mathbf{x}_w,t))$	possibly distinct roots	yes	yes
$f(t, Q(t), c(\mathbf{x}_w,t))$	possibly distinct roots	yes	yes

represent a special case of (184), the information in Table 1 is stated for the general form of (184).

The information about possible roots of equation (184) determines whether or not pulsed pumping is an option for a particular management objective chosen from one of the general classes. Notice, there are several possibilities for the roots of this equation. If the left-hand side of equation (184) becomes identically zero, then *any* set of t_i's will provide a candidate optimal pulsed pumping schedule. In this case, the problem reduces to a search of possible pumping schedules which must be further tested by the necessary and sufficient conditions of the second variation. Additionally, the possibility exists that equation (184) has no roots, which implies no t_i exists and the status of the pump should remain unchanged. Ideally, the functional classes of particular interest will have the possibility of yielding distinct roots of (184). Some specific examples of these classes are addressed in section 7.2.

Next, we examine the general classes of functionals dependent on $c_t(\mathbf{x}_w,t)$, and we find that all combinations of the independent variables of the functional in (24) might provide interesting management objectives and non-trivial pulsed pumping schedules.

7.1.2 Functionals Dependent on $c_t(\mathbf{x}_w,t)$. In this subsection, we examine the eight general classes of objective functionals that depend on the time derivative of the concentration at the extraction well. As in the previous subsection, we will examine all combinations of the independent variables of the functional in (24), and these general classes are evaluated for the possibility of using a pulsed pumping schedule.

Equation (95) is the general representation of the necessary conditions that indicate a candidate optimal pulsed pumping schedule. If all variables are present in the argument list of the objective functional (24), then the necessary conditions in (95) could be written as

$$[\hat{f} - \hat{f}_{c_t}\hat{c}_t - \hat{f}_c\hat{c} + \hat{f}_{tc_t}\hat{c} + \hat{f}_{cc_t}\hat{c}\hat{c}_t + \hat{f}_{c_tc_t}\hat{c}\hat{c}_{tt})]\Big|_{x=x_w}\Big|_{t_i+0}^{t_i-0} = 0 \tag{187}$$

for all i = 1, 2, ... n-1. Notice, with $c_t(\mathbf{x}_w,t)$ now part of the argument list of the objective functional, the roots of equation (187) are determined not only by concentration information at the extraction well, but also by information about the first and second time derivatives of the concentration, as well. Additionally, we need to know the information about the concentration and its derivatives both *before and after* the status of the pump switches from either on to off or off to on. In the cases considered in the previous subsection, we need only the concentration information at the extraction well, which is a continuous quantity. That is, concentration at the extraction well is the same for both before and after the status of the pump switches. Considering the rebound effects seen when rate-limited sorption is evident within the aquifer, we expect a discontinuity in the first and second derivatives of the concentration upon change in pump status. This presents a significant problem in implementing equation (187). This issue is discussed further in section 7.2. For the present, we examine (187) to determine the nature of the equation for different combinations in the argument list of (24).

Analysis of equation (187) leads to four separate cases for the functional in (24): (1) the functional is independent of time and concentration, (2) the functional is

independent of concentration, (3) the functional is independent of time, and (4) the functional depends on time and concentration. We see that the presence of Q(t) in the argument list of (24) does not effect any of the partial derivatives in (187), and thus leads to the four cases stated below and summarized in Table 2.

Case 1. *Functionals which are independent of time and concentration:* $f(c_t(\mathbf{x}_w,t))$ *and* $f(Q(t),c_t(\mathbf{x}_w,t)$. For this case, equation (187) becomes

$$[\hat{f} - \hat{f}_{c_t}\hat{c}_t + \hat{f}_{c_t c_t}\hat{c}\hat{c}_{tt})]\Big|_{x=x_w}\Big|_{t_i+0}^{t_i-0} = 0 \tag{188}$$

for all i = 1, 2, ... n-1.

Case 2. *Functionals which are independent of concentration:* $f(t,c_t(\mathbf{x}_w,t))$ *and* $f(t,Q(t)\ c_t(\mathbf{x}_w,t)$. For this case, equation (187) becomes

$$[\hat{f} - \hat{f}_{c_t}\hat{c}_t + \hat{f}_{tc_t}\hat{c} + \hat{f}_{c_t c_t}\hat{c}\hat{c}_{tt})]\Big|_{x=x_w}\Big|_{t_i+0}^{t_i-0} = 0 \tag{189}$$

for all i = 1, 2, ... n-1.

Case 3. *Functionals which are independent of time:* $f(c(\mathbf{x}_w,t),c_t(\mathbf{x}_w,t))$ *and* $f(Q(t),c(\mathbf{x}_w,t),c_t(\mathbf{x}_w,t))$. For this case, equation (187) becomes

$$[\hat{f} - \hat{f}_{c_t}\hat{c}_t - \hat{f}_c\hat{c} + \hat{f}_{cc_t}\hat{c}\hat{c}_t + \hat{f}_{c_t c_t}\hat{c}\hat{c}_{tt})]\Big|_{x=x_w}\Big|_{t_i+0}^{t_i-0} = 0 \tag{190}$$

for all i = 1, 2, ... n-1.

Case 4. *Functionals which depend on time and concentration:* $f(t,c(\mathbf{x}_w,t),c_t(\mathbf{x}_w,t))$ *and* $f(t,Q(t),c(\mathbf{x}_w,t),c_t(\mathbf{x}_w,t))$. For this case, equation (187) remains unchanged.

Table 2.

General Classes of Functionals Dependent on $c_t(\mathbf{x}_w,t)$.

General Class	Nature of Equation (187)	Pulsed Pumping Alternative	Interesting Objectives
$f(c_t(\mathbf{x}_w,t));f(Q(t),c_t(\mathbf{x}_w,t))$	possibly distinct roots	yes	yes
$f(t,c_t(\mathbf{x}_w,t));f(t,Q(t),c_t(\mathbf{x}_w,t))$	possibly distinct roots	yes	yes
$f(c(\mathbf{x}_w,t),c_t(\mathbf{x}_w,t))$ $f(Q(t),c(\mathbf{x}_w,t),c_t(\mathbf{x}_w,t))$	possibly distinct roots	yes	yes
$f(t,c(\mathbf{x}_w,t),c_t(\mathbf{x}_w,t))$ $f(t,Q(t),c(\mathbf{x}_w,t),c_t(\mathbf{x}_w,t))$	possibly distinct roots	yes	yes

Any of the four cases stated in Table 2 could possibly provide roots for equation (95) and produce a candidate pumping schedule, leading to an optimal solution for the optimization problem. Thus, when the time derivative of the concentration is considered in the decision making process for a management objective, the possibility exists that pulsed pumping could indeed provide an optimal pumping schedule. However, further analysis of these classes of functionals depends on the nature of the integrand of the objective functional (24).

7.1.3 Classes of Interest. So far, we have examined the objective functional (24) in the general form by considering all possible combinations of the variables t, Q(t), $c(\mathbf{x}_w,t)$, and $c_t(\mathbf{x}_w,t)$ contained in its argument list. We have seen in the previous two subsections that functionals which depend on the pumping rate and the contaminant concentration at the extraction well provide general classes which could yield a distinct solution for an optimal pulsed pumping schedule, as well as meeting desired management objectives. Additionally, when we consider the possibility of the time derivative of the

concentration as part of the management objective, we find that all combinations could yield distinct roots and lead to an optimal pulsed pumping schedule.

Further analysis of any of the equations (184), (187), (188), (189), or (190) requires some assumptions about the specific nature of the integrand f. First, we should consider what variables are likely to be present in any particular management objective. Also, we need to assume how the variables will occur in the objective, e.g. as products of polynomials, in exponentials, in the denominator of the integrand, etc. With these limiting assumptions, we can further analyze the equations which produce an optimal schedule, and demonstrate the usefulness of this optimization technique through the use of the simulation model SUTRA.

In the next section of this chapter, we will present specific examples from two general classes and demonstrate how to determine a candidate pulsed pumping schedule. First, we examine objective functionals which depend on time, the pumping rate, and the contaminant concentration at the extraction well. We will assume that the integrand of the functional is analytic in $c(s,t)$, leading to a power series representation for $f(t,Q(t),c(s,t))$, where the coefficients of the powers of $c(s,t)$ depend on t and $Q(t)$. Next, we add the time derivative of the concentration to the integrand and make a simplifying assumption for the relationship between the first and second time derivatives of the concentration on successive intervals, leading to another example of the technique.

7.2 *Examples*

Suppose the integrand of (24) is independent of the time derivative of the concentration and is an analytic function in the concentration. Then we can write

$$f(t,Q,c)=\sum_{k=0}^{\infty}a_k(t,Q)c^k, \tag{191}$$

where the coefficients a_k might depend upon time and the pumping rate. Substituting this representation for the integrand into the functional in (24), equation (95) becomes

$$\begin{aligned}\left[\hat{f}-\hat{c}\hat{f}_c\right]\Big|_{x=x_w}\Big|_{t_i+0}^{t_i-0} &= \left[\sum_{k=0}^{\infty}a_k(t,\hat{Q}(t))\hat{c}^k(\mathbf{x}_w,t)-\hat{c}(\mathbf{x}_w,t)\sum_{k=0}^{\infty}a_k(t,\hat{Q}(t))k\hat{c}^{k-1}(\mathbf{x}_w,t)\right]\Big|_{t_i+0}^{t_i-0}\\ &= \left[a_0(t,\hat{Q}(t))+\sum_{k=2}^{\infty}a_k(t,\hat{Q}(t))(1-k)\hat{c}^k(\mathbf{x}_w,t)\right]\Big|_{t_i+0}^{t_i-0}=0\end{aligned} \tag{192}$$

for all i = 1, 2, ... n-1. From (192), we see that if we wish to represent the integrand of (24) as a product of a polynomial function in the concentration and any function which depends on the time and the pumping rate, then the concentration polynomial must have degree greater than one. That is, if we choose to let

$$f(t,Q,c)=a_0(t,Q)+a_1(t,Q)c$$

then equation (192) becomes

$$\left[\hat{f}-\hat{c}\hat{f}_c\right]\Big|_{x=x_w}\Big|_{t_i+0}^{t_i-0}=a_0(t,\hat{Q}(t))\Big|_{t_i+0}^{t_i-0}=0. \tag{193}$$

for all i = 1, 2, ... n-1. Table 1 indicates that roots of (193) may be found, but are unlikely to lead to optimal solutions for any interesting management objectives. The following example illustrates a common management goal in this category of functionals. This particular example has received a large amount of attention in the literature (Voudrias & Yea, 1994; Rabideau & Miller, 1994; Harvey et al., 1994). We find that because of the linearity of the concentration term in the proposed objective functional, pulsed pumping will not afford an optimal pumping schedule.

Example 1: Maximize the amount of contaminant mass removed while minimizing the amount of water mass removed over a finite time interval. This problem can be formalized as a minimization problem:

$$\text{Minimize} \qquad J[Q,c] = (1-z)\int_0^{t_f}\int_{\Gamma_1} \rho_w Q(t)ds_1dt - z\int_0^{t_f}\int_{\Gamma_1} Q(t)c(s,t)ds_1dt, \qquad (194)$$

constrained by the appropriate conditions depicted by (25) - (27), where ρ_w is the density of the water [M/L^3] and z is a weighting factor [dimensionless] ($0 < z < 1$) introduced because of the large difference between mass of contaminant and mass of fluid pumped out of the aquifer (Hartman, 1994). For the functional in (194), we have

$$f(t,Q,c) = (1-z)\rho_w Q - zQc,$$

and equation (192) becomes

$$\left[\hat{f} - \hat{c}\hat{f}_c\right]\Big|_{x=x_w}\Big|_{t_i+0}^{t_i-0} = (1-z)\rho_w\hat{Q}(t)\Big|_{t_i+0}^{t_i-0} = 0 \qquad (195)$$

for all i = 1, 2, ... n-1. Obviously, equation (195) can never have roots and a candidate optimal pulsed pumping schedule does not exist, and thus all that is left is to decide whether the pump is always on or always off. If the pump is always off, then $Q(t) \equiv 0$, and equation (194) becomes $J[0,c] \equiv 0$. If the pump is always on, then the decision to pump is determined by the weighting factor z, in equation (194). That is, let $Q(t) = Q_{ON}$ for all time, then equation (194) becomes

$$J[Q_{ON},c] = Q_{ON} t_f \left[(1-z)\rho_w - \frac{z}{t_f} \int_0^{t_f} c(\mathbf{x}_w, t)dt \right], \tag{196}$$

and the sign of (196) determines the status of the pump. If $J[Q_{ON},c]$ in equation (196) is less than zero, then $J[Q_{ON},c]$ represents a minimum for the functional and the decision is to pump continuously. If $J[Q_{ON},c]$ is greater than zero, then $J[0,c] = 0$ represents a minimum for the functional and the decision is to leave the pump idle. Closer examination of (194) and (196) shows that as z approaches the value 1, a greater emphasis is placed on maximizing the mass of contaminant removed and the decision is to pump continuously. If z approaches zero, then the emphasis is placed on minimizing the mass of water removed and the decision is not to pump. □

A number of research efforts (Voudrias & Yea, 1994; Rabideau & Miller, 1994; Harvey et al., 1994) have sought to optimize remediation goals which could be described by the objective functional in Example 1. Their studies included numerous runs of simulations that tested the theory of pulsed pumping by using "best-guess" techniques to determine an optimal pulsed pumping schedule. As was demonstrated in Example 1,

these investigations could not find an optimal pulsed pumping schedule, because a schedule which optimizes the functional in (194) does not exist. Comparison of these studies with the current work illustrates the power of this variational approach. By setting the problem as the optimization of an objective functional, rigorous results are obtained which obviate the need for trial-and-error searches of solution spaces. This approach also encourages examination of what features are truly desired in the management functional. The next example illustrates that the functional in Example 1, which accurately represents the management goal most prevalent in the literature, may not, in fact, be the best choice.

Example 1 illustrates the need to alter the nature of the objective functional, while maintaining a meaningful objective, to produce an optimal pulsed pumping schedule. Tables 1 and 2 indicate that a pulsed pumping schedule could be derived which optimizes a meaningful objective, either by introduction of higher degree terms in the concentration (for functionals of the type represented by equation (191)) or by introduction of information about the time derivative of the concentration at the extraction well, The next two examples examine both of these possibilities.

The next example demonstrates how a functional whose integrand has a factor that is a polynomial in the concentration with degree 3 yields a candidate pulsed pumping schedule, which, in turn, is further tested by the necessary and sufficient conditions of the second variation. The concentration information at the extraction well is provided by the modified SUTRA model which incorporates rate-limited sorption (Caspers, 1994). Before we pursue this example, we define a function referred to as the *essential concentration function*.

Definition 7. Let c_S represent the acceptable drinking water standard of a contaminant concentration within a solute. The *essential concentration function*, $\mathcal{E}(c)$, is defined as any function of the concentration at the extraction well, such that $\mathcal{E}(c)$ is positive for all concentrations above c_S (referred to as essential concentrations), and $\mathcal{E}(c)$ is negative for all concentrations below c_S (referred to as non-essential concentrations). Further, $\mathcal{E}(c_S) = \mathcal{E}(0) = 0$ and the units of $\mathcal{E}(c)$ are contaminant mass per volume of the water phase [M/L^3]. See Figure 12 for an example of $\mathcal{E}(c)$.

By using the essential concentration function, we could easily define an objective functional which maximizes the (time) averaged essential concentration removed at the extraction well, but also minimizes the (time) averaged non-essential concentration removed. That is, we maximize the high concentrations, and minimize the low concentrations. Notice, in example 1, the essential concentration function was $\mathcal{E}(c) = c$, and thus *all concentrations* are essential which implies that the drinking water standard is

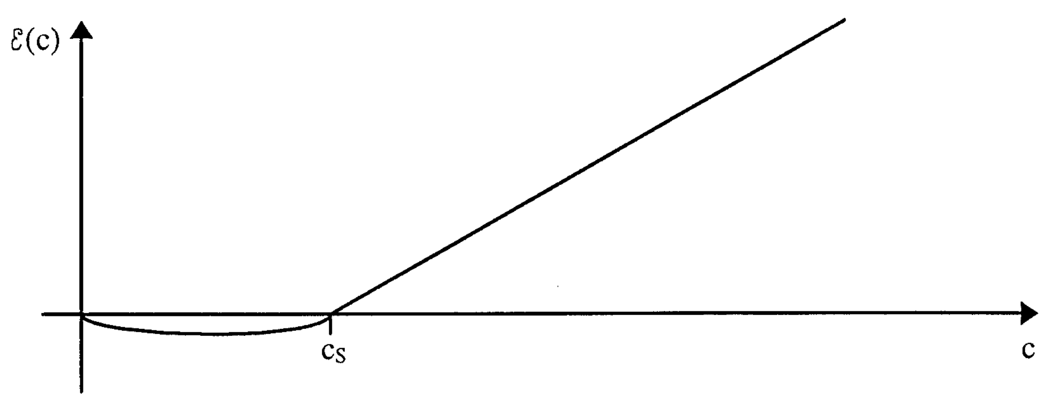

Figure 12. An example of an essential concentration function.

$c_S = 0$. For most contaminated aquifers, a goal which returns the aquifer to a pristine condition is neither feasible nor practical, and as such, the objective of Example 1 is not realistic.

Example 2 applies the definition of essential concentration to develop a pulsed pumping schedule for a more realizable objective functional. Example 3 pursues another possibility for the objective functional by introducing time derivative information for the concentration into the objective.

Example 2: Maximize the essential mass removed while minimizing the non-essential mass removed and the total mass of the water removed, where the essential mass function is determined by some prescribed drinking water standard, $c_S > 0$. Before we state our specific optimization problem, we first observe that our definition of essential concentration makes the integrand of J[Q,c] independent of the time derivative of the concentration, and the objective functional has the form of equation (183). Additionally, the essential concentration function was chosen such that equation (184) produced a non-trivial pulsed pumping schedule which meets the objectives of this example.

In the analysis of this problem, we find that Theorems 9 and 10 must be modified to reflect the independence of the time derivative of the concentration at the well. First, notice the terms in (125) can be written as

$$P^{(i)}(t) = 0, \qquad\qquad R^{(i)}(t) = \frac{1}{2} f_{cc}[t, \hat{Q}^{(i)}(t), \hat{c}^{(i)}(\mathbf{x}_w, t)],$$

$$m_{11}^{(i)} = -\frac{1}{2}\left[\hat{f}_c \hat{c}_t\right]_{x=x_w}\Big|_{t_i+0}^{t_i-0}, \qquad m_{12}^{(i)} = m_{21}^{(i)} = \frac{1}{2}\left[\hat{f}_c\right]_{x=x_w}\Big|_{t_i+0}^{t_i-0}, \quad \text{and} \qquad m_{22}^{(i)} = 0,$$

so that the second variation of the Lagrangian becomes

$$\delta^2 \mathcal{L}[\hat{Q},\hat{c},\hat{\lambda};\Delta t_i, h, \mu] = \int_0^{t_f} R(t) h^2 dt + \sum_{i=1}^{n-1} [\Delta t_i \quad \delta c_i] \cdot \begin{bmatrix} m_{11}^{(i)} & m_{12}^{(i)} \\ m_{21}^{(i)} & 0 \end{bmatrix} \cdot \begin{bmatrix} \Delta t_i \\ \delta c_i \end{bmatrix},$$

and thus, the statement in the hypothesis of both Theorems 9 and 10 that $P(t) > 0$ for all t becomes $R(t) > 0$ over the same time interval. Notice also, the matrix $\mathbf{M}^{(i)}$ above will always have a negative determinant, which makes it impossible for $\mathbf{M}^{(i)}$ to be a nonnegative definite matrix. Thus, the product $\overline{\Delta}_i^{\,T} \cdot \mathbf{M}^{(i)} \overline{\Delta}_i$ will always be nonpositive. This hinders the analysis if we seek to minimize a functional, since we are no longer assured that the second variation is positive definite, as in Theorem 9. However, if we seek to maximize a functional, Theorems 9 and 10 are still usable if we use the following revised theorems.

Theorem 9 (REVISED). The quadratic functional

$$A[h, \Delta t_i, \delta c_i] = \int_{t_{i-1}}^{t_{i+1}} R(t) h^2 dt + \overline{\Delta}_i^T \cdot \mathbf{M}^{(i)} \cdot \overline{\Delta}_i, \tag{197}$$

where $\overline{\Delta}_i^T = [\Delta t_i \quad \delta c_i]$, and

$$R(t) = \begin{cases} R^{(i)}(t) & t_{i-1} < t < t_i \\ R^{(i+1)}(t) & t_i < t < t_{i+1} \end{cases},$$

such that $R(t) < 0$ for all $t \in (t_{i-1}, t_i) \cup (t_i, t_{i+1})$, and $\mathbf{M}^{(i)}$ is a nonpositive definite matrix (denoted by $\mathbf{M}^{(i)} \le 0$), is a negative definite functional for all $h(t)$ such that $h(t_{i-1}) = 0$ $h(t_{i+1}) = 0$ if and only if the interval $[t_{i-1}, t_{i+1}]$ contains no conjugate times to t_{i-1}.

Theorem 10 (REVISED). Suppose that for some admissible functions $(\hat{Q}, \hat{c}, \hat{\lambda})$ the Lagrangian for the optimization problem defined by (183) and (25) - (27) satisfies the following conditions:

1. The functions $(\hat{Q}, \hat{c}, \hat{\lambda})$ are an extremal, and hence the first variation of the Lagrangian vanishes; implying that the conditions stated in (75), (78), (81), (83), (84), (89), (91), and (95) are met (Note: $\hat{f}_{c_t} \equiv 0$ in these conditions).

2. For the functions $(\hat{Q}, \hat{c}, \hat{\lambda})$,

$$R^{(i)}(t) \equiv \frac{1}{2} f_{cc}[t, \hat{Q}^{(i)}(t), \hat{c}^{(i)}(\mathbf{x}_w t)] < 0 \tag{198}$$

for all $t \in [t_{i-1}, t_i]$, and for all $i = 1, 2, \ldots n$, and

$$\mathbf{M}^{(i)} \leq 0 \tag{199}$$

for all $i = 1, 2, \ldots n$-1, where $\mathbf{M}^{(i)}$ is given as

$$\mathbf{M}^{(i)} = \frac{1}{2} \begin{bmatrix} -\hat{f}_c \hat{c}_t \Big|_{t_i+0}^{t_i-0} & \hat{f}_c \Big|_{t_i+0}^{t_i-0} \\ \hat{f}_c \Big|_{t_i+0}^{t_i-0} & 0 \end{bmatrix}_{\mathbf{x}=\mathbf{x}_w}$$

and

$$m_{11}^{(i)} = -\frac{1}{2} \left[\hat{f}_c \hat{c}_t \right]_{\mathbf{x}=\mathbf{x}_w} \Big|_{t_i+0}^{t_i-0} \leq 0.$$

3. The time interval $[t_{i-1}, t_{i+1}]$, contains no times which are conjugate to the time t_{i-1}, for all $i = 1, 2, \ldots n$.

Then the functional in (183), constrained by the conditions in (25) - (27) has a maximum at $(\hat{Q}, \hat{c}, \hat{\lambda})$ with respect to $\|*\|_{\bar{1}}$.

This problem can now be formalized as a maximization problem:

Maximize $$J[Q,c] = \int_0^{t_f}\int_{\Gamma_1} f(t,Q(t),c(s,t))ds_1dt, \tag{200}$$

constrained by the appropriate conditions depicted by (25) - (27), where

$$f(t,Q,c) = -(1-z)\rho_w[Q+Q_{LO}] + z\mathcal{E}(c)[Q+Q_{LO}] \tag{201a}$$

and

$$\mathcal{E}(c) = \eta(\sigma c)^2 + \upsilon(\sigma c)^3. \tag{201b}$$

In equations (201), ρ_w is the density of the water [M/L^3] and z is a weighting factor [dimensionless] ($0 < z < 1$) introduced because of the large difference between mass of contaminant and mass of fluid pumped out of the aquifer, η and υ are constants which are chosen to satisfy some drinking water standard for the contaminant [M/L^3], σ is a concentration scaling factor [L^3/M] such that (σc) represents the scaled, dimensionless concentration, and Q_{LO} is a reduced pumping rate, introduced to maintain hydraulic control of the contaminant plume [L^3/T].

Notice, in equation (201b), the essential concentration function is a cubic polynomial with the coefficients of the constant term and the linear terms set to zero. The choice of a cubic was necessary to ensure that $\mathcal{E}(c)$ has a zero corresponding with the concentration standard, c_S (see Figure 12). Further, notice that equation (201) could be written as

$$f(t,Q,c) = \left[(z-1)\rho_w + z\eta(\sigma c)^2 + z\upsilon(\sigma c)^3\right][Q+Q_{LO}],$$

or, alternatively as

$$f(t,Q,c) = \left[K_0 + K_2(\sigma c)^2 + K_3(\sigma c)^3\right]\left[Q + Q_{LO}\right],$$

where K_0, K_2, are K_3, are constants. With this representation for the integrand, we see that f in equation (201) is analytic in c(s,t) and thus, if the functions $(\hat{Q},\hat{c},\hat{\lambda})$ are an extremal, they must satisfy the necessary conditions in (192). As we noted previously, the linear term of f vanishes in equation (192) and any constant term would become part of K_0 above, so the choice of $\mathcal{E}(c)$ in (201b) is justified. Thus, the NOC of (192) becomes

$$\begin{aligned}
&\left[\hat{f} - \hat{c}\hat{f}_c\right]\Big|_{x=x_w}\Big|_{t_i+0}^{t_i-0} = \\
&\quad\Big\{\left[K_0 + K_2(\sigma\hat{c})^2 + K_3(\sigma\hat{c})^3\right]\cdot\left[\hat{Q}^{(i)} + Q_{LO}\right] \\
&\qquad\qquad - \hat{c}\left[2K_2\sigma^2\hat{c} + 3K_3\sigma^3\hat{c}^2\right]\cdot\left[\hat{Q}^{(i)} + Q_{LO}\right]\Big\}_{\hat{c}=\hat{c}^{(i)}} \\
&\quad -\Big\{\left[K_0 + K_2(\sigma\hat{c})^2 + K_3(\sigma\hat{c})^3\right]\cdot\left[\hat{Q}^{(i+1)} + Q_{LO}\right] \\
&\qquad\qquad - \hat{c}\left[2K_2\sigma^2\hat{c} + 3K_3\sigma^3\hat{c}^2\right]\cdot\left[\hat{Q}^{(i+1)} + Q_{LO}\right]\Big\}_{\hat{c}=\hat{c}^{(i+1)}} = 0
\end{aligned} \tag{202}$$

for all i = 1, 2, ... n-1, and the roots of (202) provide the candidate pulsed pumping schedule. Suppose the extraction pump is initially on, and we wish to find the time t_1 to turn the pump off. Then, for this first pumping interval we must satisfy

$$\begin{aligned}
&\Big\{\left[K_0 + K_2(\sigma\hat{c})^2 + K_3(\sigma\hat{c})^3\right]\cdot\left[Q_{ON} + Q_{LO}\right] - \hat{c}\left[2K_2\sigma^2\hat{c} + 3K_3\sigma^3\hat{c}^2\right]\cdot\left[Q_{ON} + Q_{LO}\right]\Big\}_{\hat{c}=\hat{c}^{(1)}} \\
&\quad -\Big\{\left[K_0 + K_2(\sigma\hat{c})^2 + K_3(\sigma\hat{c})^3\right]\cdot Q_{LO} - \hat{c}\left[2K_2\sigma^2\hat{c} + 3K_3\sigma^3\hat{c}^2\right]\cdot Q_{LO}\Big\}_{\hat{c}=\hat{c}^{(2)}} = 0.
\end{aligned} \tag{203}$$

Since $\hat{c}$ is continuous at $t = t_1$, then $\hat{c}^{(1)} = \hat{c}^{(2)}$ and the candidate switching time is the first zero of the function G(t), stated as

$$G(t) = \left[K_0 - K_2(\sigma\hat{c})^2 - 2K_3(\sigma\hat{c})^3\right], \tag{204}$$

where $\hat{c} = \hat{c}^{(1)}(\mathbf{x}_w, t_1)$, and the concentration information at the well could be provided by any contaminant transport model which incorporates first-order, rate-limited sorption with the extraction well on. Notice, if we wish to find the next time to turn the pump on, then the zero of G(t) again provides the candidate switching time, however now the concentration information is provided by the model with the extraction well turned off.

Caspers (1994) developed a modified SUTRA code which successfully incorporates first- and second-order diffusion models which emulate rate-limited sorption into a two-dimensional finite element flow and transport model. For the present example, Caspers' code with typical input parameters was used to generate concentration information at the extraction well, which was placed in a hypothetical two-dimensional, contaminated, sandy aquifer (Caspers, 1994:Ch 4). The first-order diffusion model was used with a rate constant $\alpha = 0.005$ day^{-1}. Initial contaminant was simulated by injection of carbon tetrachloride into the aquifer at a rate of 5 m^3/day, with a concentration of 5.0 μg/l, for a period of 100 days. Following this initial injection, the system was undisturbed for an additional 365 days and transient solute transport was simulated. The cleanup period followed, and the extraction well operated at a pumping rate of 400 m^3/day during active intervals.

To determine the zeroes of G(t), Caspers' model was run for 200 days and concentration samples were taken once per day. Using these 200 discrete data points, we sought to find the time that the expression in (204) goes to zero. For this example, we used a weighting factor of z = 0.9982, concentration scaling factor of $\sigma = 10^{10}$ m^3/kg, and

a water density of $\rho_w = 1000$ kg/m^3. The essential concentration function was determined to meet a cleanup standard of 120 ppb (parts per billion). Notice, if we set the essential concentration function to zero, we can write

$$\mathcal{E}(c) = (\sigma c)^2[\eta + \upsilon(\sigma c)] = 0,$$

and the zeroes of $\mathcal{E}(c)$ are at $c = 0$ and $c = \frac{-\eta}{\upsilon\sigma}$. If we let $c_S = \frac{-\eta}{\upsilon\sigma}$, we can choose constants $\eta = -1.2$ and $\upsilon = 0.001$ to satisfy Definition 7 for a cleanup standard of $c_S = 120$ ppb. For these values of the constants in (201), the constants in (204) become: $K_0 = -1.8$, $K_2 = -1.2$, and $K_3 = 0.001$ and a graph of the function G(t) is presented in Figure 13.

From the graph in Figure 13, we see that the first time to shut off the pump occurs on day 83 of the first pumping interval. With this knowledge, we ran Caspers' code again, but only to simulate extraction for 83 days. At the end of this simulation, the final

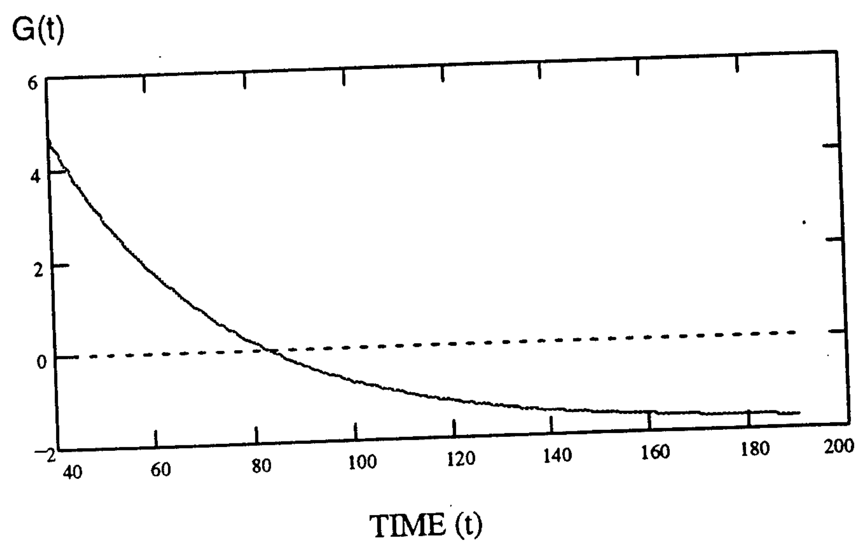

Figure 13. Plot of G(t) for 200 data points, extraction pump on.

concentration information serves as the initial concentration distribution for the first idle pumping interval. Concentration information for this idle interval is found again by using Caspers' code, only now the pumping rate is set to zero. Again, we sample the concentration at the well for 200 days and use these discrete data points to find the time t_2, the first time to turn the pump back on (Figure 14).

From Figure 14, we determine that the time to restart the pump occurs on day 21 of the first idle interval. Again, we ran Caspers' code for 21 days to find the initial contaminant concentration distribution for the next pumping interval, and then started the simulation again to determine the next time to shut the pump off again. This process was continually repeated to determine the optimal candidate pulsed pumping schedule for the duration of the cleanup project. For this example, the procedure was carried out to determine the next pump-off and pump-on times, t_3 and t_4, and the results are summarized in Table 3.

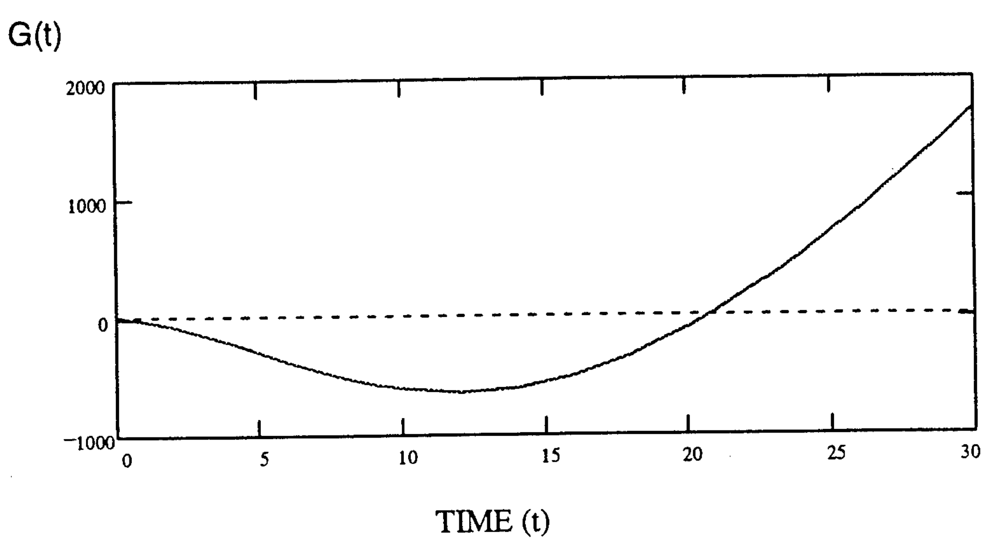

Figure 14. Plot of G(t) for 30 data points, extraction pump off.

Next, we need to demonstrate that the candidate optimal pumping schedule presented in Table 3 does indeed represent a maximum solution for the functional stated in (200) and (201). To accomplish this, we examine the term $R^{(i)}(t)$ of Theorem 10 (Revised) for all $t \in [t_{i-1}, t_i]$, and for i = 1, 2, 3, and 4, and the term $\mathbf{M}^{(i)}$ for i = 1, 2, 3, and 4, in particular the m_{11} terms of each matrix $\mathbf{M}^{(i)}$.

According to Theorem 10 (Revised), we need $R^{(i)}(t)$ to be negative on the i^{th} interval for every i. For the particular functional we are considering here, the inequality condition in (198) becomes

$$f_{cc}[t, \hat{Q}^{(i)}(t), \hat{c}(\mathbf{x}_w, t)] = 2\sigma^2[K_2 + 3K_3(\sigma\hat{c})] \cdot [\hat{Q}^{(i)}(t) + Q_{LO}] < 0 \tag{205}$$

for all $t \in [t_{i-1}, t_i]$, and for i = 1, 2, 3, and 4. If Q_{LO} is chosen to be a small positive constant, then the constraint in (205) becomes

$$[K_2 + 3K_3(\sigma\hat{c})] < 0 \tag{206}$$

for all $t \in [t_{i-1}, t_i]$, and for i = 1, 2, 3, and 4.

Table 3.

Switching Times and Observed Concentrations (Example 2).

Switching Time	Day of Project	Observed Concentration
t_0	0	1.57×10^{-8}
t_1	83	1.24×10^{-10}
t_2	104	6.05×10^{-9}
t_3	119	1.10×10^{-10}
t_4	158	6.04×10^{-9}

Since the concentration at the extraction well is a continuous, monotone function throughout the i^{th} interval for any i, then the inequality in (206) is satisfied throughout the interval if it is satisfied at the endpoints. For instance, for the first interval (i = 1) the inequality at the endpoints becomes

$$[-1.2 + 3(0.001)(\sigma\hat{c}_0)] = -0.726 < 0 \qquad (207a)$$

and

$$[-1.2 + 3(0.001)(\sigma\hat{c}_{83})] = -1.196 < 0. \qquad (207b)$$

Similarly, the inequality in (206) is found to hold when i = 2, 3, and 4 as well, so that the only test which remains is to verify that $\mathbf{M}^{(i)} \leq 0$ for i = 1, 2, 3, and 4.

Again, since we know the determinant of $\mathbf{M}^{(i)}$ is always negative, then inequality (199) holds if the m_{11} term is negative or zero for each i. For example, when i = 1

$$m_{11}^{(1)} = -\frac{1}{2}\left[\hat{f}_c\hat{c}_t\right]_{x=x_w}\Big|_{t_1+0}^{t_1-0} = -\frac{1}{2}\left[2K_2\sigma^2\hat{c} + 3K_3\sigma^3\hat{c}^2\right]\cdot\left[\hat{Q}(t) + Q_{LO}\right]\hat{c}_t\Big|_{x=x_w}\Big|_{t_1+0}^{t_1-0}, \qquad (208)$$

which becomes

$$m_{11}^{(1)} = -\frac{\sigma^2\hat{c}}{2}\left[2K_2 + 3K_3(\sigma\hat{c})\right]\cdot\left[\left(Q_{ON} + Q_{LO}\right)\hat{c}_t^- - Q_{LO}\hat{c}_t^+\right]\Big|_{x=x_w}, \qquad (209)$$

where $\hat{c}_t^-$ and $\hat{c}_t^+$ represent the derivative of the concentration at the extraction well just before and just after the status of the pump switches from on to off, respectively. Plugging in the value for $\hat{c}(\mathbf{x}_w, t_1) = \hat{c}_{83}$ from Table 3, and assuming $\hat{c}_t^- < 0$ and $\hat{c}_t^+ > 0$ (since the concentration is decreasing on interval 1, and increasing on interval 2), we find

that (209) is negative for the given constants. In fact, the $m_{11}^{(i)}$ term is found to be negative for each i = 1, 2, 3, and 4, and thus by *Sylvester's criterion* the matrix $\mathbf{M}^{(i)}$ is nonpositive for i = 1, 2, 3, and 4.

Returning to Theorem 9 (Revised), since R(t) is negative for all $t \in (t_{i-1}, t_i) \cup (t_i, t_{i+1})$, and $\mathbf{M}^{(i)}$ is a nonpositive definite matrix, then the functional A in (197) is always negative. Thus, A is a negative definite functional for all h(t) such that $h(t_{i-1}) = 0$ and $h(t_{i+1}) = 0$, and according to the theorem, the interval $[t_{i-1}, t_{i+1}]$ contains no conjugate times to t_{i-1} for every i. With this statement, we have satisfied all the conditions stated in Theorem 10 (Revised), and as such the pumping schedule $(t_1, t_2, t_3, t_4, \ldots)$ represents an optimal pumping solution which maximizes the functional defined by (200) and (201), constrained by the appropriate conditions of (25) - (27). □

From Example 2, we clearly see the potential for the optimization technique presented in this document. The definition of the essential concentration function could easily be tied into a remediation cost function for a particular cleanup site. That is, we can think of $\mathcal{E}(c)$ as a penalty function that attaches a greater cost to remediating water which already meets a prescribed standard. Further, from this example we see that the conditions stated in Theorem 10 (or Revised Theorem 10) are easy to test for any particular functional. Finally, implementation at an operational facility could easily incorporate the actual concentration information, or at least the information could be provided by a validated numerical model (required at remediation sites by regulation) which accurately predicts the contaminant concentration.

The next example again illustrates how this optimization method can be used, only this example assumes the objective functional depends on the time derivative of the concentration at the extraction well. The idea behind Example 3 is that a remediation site operates more efficiently if, during the active pumping intervals, the pump withdraws contaminated water at a steady contaminant concentration level. Treating for a steady level of contaminant alleviates the need to retool the air-scrubbers at the site to handle wide ranges of contaminant concentrations. By minimizing the rate at which the contaminant concentration changes, while also minimizing the mass of the water withdrawn, we can assure that retooling costs will be held to a minimum.

Example 3: Minimize the rate at which contaminant concentration is changing, while also minimizing the mass of contaminated water withdrawn. We state the optimization problem for this example as:

<u>Minimize</u>:
$$J[Q,c] = \int_0^{t_f}\int_{\Gamma_1} f(t,Q(t),c_t(s,t))ds_1dt, \tag{210}$$

constrained by the appropriate conditions depicted by (25) - (27), where

$$f(t,Q(t),c_t(s,t)) = (1-z)\rho_w[Q(t)+Q_{LO}] + z\frac{1}{2}(\sigma c_t)^2[Q(t)+Q_{LO}], \tag{211}$$

where the constants in (211) are the same as those introduced in Examples 1 and 2, except we have used $z = 0.999925$ for this example and the 1/2 is introduced for convenience. Notice, the integrand depicted by (211) is independent of the concentration at the extraction well. For this particular class of functionals, equation (188) provides the

candidate pulsed pumping schedule. Further, the matrix $\mathbf{M}^{(i)}$ of Theorem 10 reduces to the $m_{11}^{(i)}$ term for each i = 1, 2, ... n-1, so that condition (174) becomes

$$m_{11}^{(i)} = -\frac{1}{2}\left[\hat{f}_{c_t}\hat{c}_{tt}\right]_{x=x_w}\Big|_{t_i+0}^{t_i-0} \geq 0 \tag{212}$$

for all i = 1, 2, ... n-1.

Suppose the functions $(\hat{Q},\hat{c},\hat{\lambda})$ are an extremal for the functional in (210) and (211), and let $K_1 = (1-z)\rho_w$ and $K_2 = \dfrac{z}{2}$, then the necessary conditions in (188) which generate the candidate optimal pumping schedule become

$$\begin{aligned}[\hat{f} - \hat{f}_{c_t}\hat{c}_t + \hat{f}_{c_t c_t}\hat{c}\hat{c}_{tt})]\Big|_{x=x_w}\Big|_{t_i+0}^{t_i-0} &= \left[\hat{Q}^{(i)} + Q_{LO}\right]\left(K_1 - K_2(\sigma\hat{c}_t)^2 + 2K_2\sigma^2\hat{c}\hat{c}_{tt}\right)_{\hat{c}=\hat{c}^{(i)}} \\ &\quad - \left[\hat{Q}^{(i+1)} + Q_{LO}\right]\left(K_1 - K_2(\sigma\hat{c}_t)^2 + 2K_2\sigma^2\hat{c}\hat{c}_{tt}\right)_{\hat{c}=\hat{c}^{(i+1)}} = 0\end{aligned} \tag{213}$$

for all i = 1, 2, ... n-1, and the roots of (213) provide the candidate schedule. As in the previous example, suppose the extraction pump is initially on, and we wish to find the time t_1 to turn the pump off. Since $\hat{c}$ is continuous at t = t_1, then $\hat{c}^{(1)} = \hat{c}^{(2)}$ and the candidate switching time must satisfy

$$\begin{aligned}&\left[Q_{ON} + Q_{LO}\right]\left(K_1 - K_2(\sigma\hat{c}_t^-)^2 + 2K_2\sigma^2\hat{c}\hat{c}_{tt}^-\right) \\ &\qquad - Q_{LO}\left(K_1 - K_2(\sigma\hat{c}_t^+)^2 + 2K_2\sigma^2\hat{c}\hat{c}_{tt}^+\right) = 0,\end{aligned} \tag{214}$$

where $\hat{c} = \hat{c}^{(1)}(\mathbf{x}_w, t_1)$ and $\hat{c}_t^-$, $\hat{c}_{tt}^-$, $\hat{c}_t^+$, and $\hat{c}_{tt}^+$ are the first and second time derivatives of the concentration at the extraction well, with the minus sign representing the value just *before* the pump is turned off and the plus sign representing the value just *after* the pump

is turned off. As we stated earlier (sub-section 7.1.2), the rebound effects (expected when rate-limited sorption is evident within an aquifer) lead to discontinuities in the first and second time derivatives of the concentration. Previous results (Caspers, 1994:Ch 4) show the concentration will rebound as seen in Figure 15, and as such, we assume $\hat{c}_t^- < 0$, $\hat{c}_{tt}^- > 0$, and $\hat{c}_t^+ > 0$, $\hat{c}_{tt}^+ < 0$. Additionally, since we have no knowledge of the exact magnitudes of the derivative terms after the pump is switched (without actually switching it), we make the following assumptions: $\hat{c}_t^+ = \kappa_1 \hat{c}_t^-$ and $\hat{c}_{tt}^+ = \kappa_2 \hat{c}_{tt}^-$, where κ_1 and κ_2 are unknown negative constants, which could be approximated by running numerous simulations to predict the rate of rebound. For the purpose of this illustration, we choose these constants arbitrarily to be: $\kappa_1 = -4.5$ and $\kappa_2 = -2$, which imply that the concentration is increasing rapidly the instant the pump is turned off and that the concavity has changed as depicted in Figure 15. With these assumptions, the candidate pulsed pumping schedule is derived from the zeroes of H(t), given as

$$H(t) = A_1 + A_2\left(\sigma \hat{c}_t\right)^2 + A_3\left(\sigma^2 \hat{c}\hat{c}_{tt}\right), \tag{215}$$

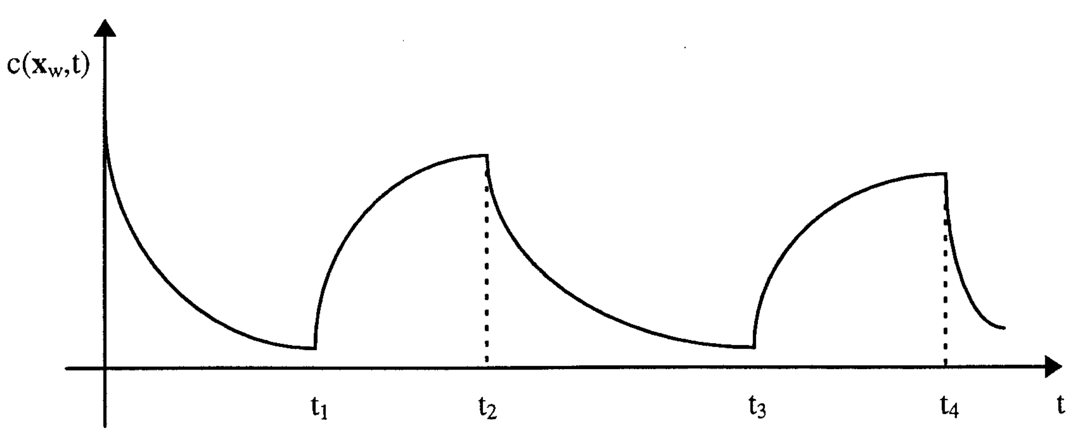

Figure 15. Tailing and rebound effects seen at the extraction well.

where $\hat{c} = \hat{c}^{(1)}(\mathbf{x}_w, t_1)$, $\hat{c}_t = \hat{c}_t^-$, $\hat{c}_{tt} = \hat{c}_{tt}^-$, and the constants A_1, A_2, and A_3 in (215) are combinations of the constants used in this example, produced by (214). The values of $K_1 = 0.075$, $K_2 = 0.5$, $Q_{ON} = 400$, and $Q_{LO} = 20$ produced the constants $A_1 = 30$, $A_2 = -103$, and $A_3 = 430$ in equation (215).

To determine the zeroes of H(t) in (215), we again ran Caspers' model for 200 days and concentration samples were taken once per day. Using these 200 discrete data points, we seek to find the first time H(t) goes to zero. Notice, for this example we need not only the concentration information, but also the first and second time derivative information as well. Numerical differentiation with a three-point formula was used to approximate the value of the first derivative at each sample point. The formula used current concentration information along with the information from two successive samples to make the approximation. Similarly, the second derivative was approximated using a three-point formula in conjunction with the first derivative approximations at each data point. A graph of H(t) is presented in Figure 16.

From the graph in Figure 16, we see that the first time to shut off the pump occurs on day 18 of the first pumping interval. Continuing this procedure, as in Example 2, the information from day 18 serves as the initial data for the first pump-off interval. Figure 17 presents a graph of H(t) where discrete concentration information comes from Caspers' code with the pumping rate set to zero, and we see the first time to resume pumping occurs on day 13 of the idle pumping interval. This process was continually repeated to determine the optimal candidate pulsed pumping schedule for the duration of

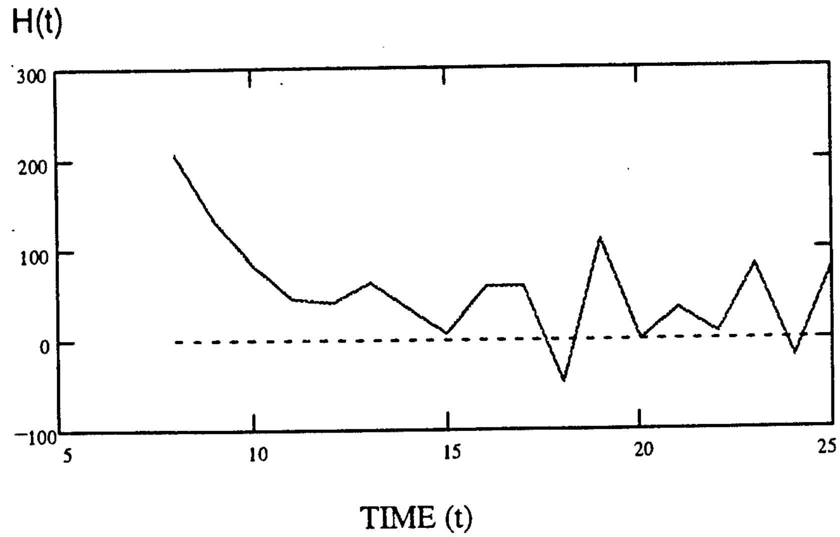

Figure 16. Plot of H(t) for 25 data points, extraction pump on.

cleanup project. For this example, the procedure was carried out to determine the next pump-off and pump-on times, t_3 and t_4, and the results are summarized in Table 4.

Next, we need to demonstrate that the candidate optimal pumping schedule presented in Table 4 does indeed represent a minimum solution for the functional stated

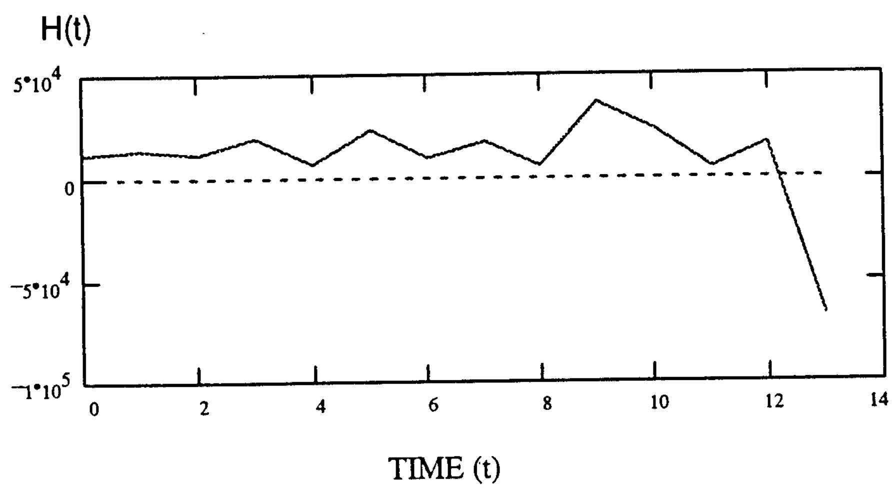

Figure 17. Plot of H(t) for 13 data points, extraction pump off.

Table 4.

Switching Times and Observed Concentrations (Example 3).

Switching Time	Day of Project	Observed Concentration
t_0	0	1.57×10^{-8}
t_1	18	3.33×10^{-10}
t_2	31	1.15×10^{-8}
t_3	45	2.21×10^{-10}
t_4	61	8.94×10^{-9}

in (210) and (211). To accomplish this, we need to examine the term $P^{(i)}(t)$ of (173) for all $t \in [t_{i-1}, t_i]$, and for i = 1, 2, 3, and 4, and the $m_{11}^{(i)}$ term for i = 1, 2, 3, and 4.

According to Theorem 10, we need $P^{(i)}(t)$ to be negative on the i^{th} interval for every i. For the particular functional we are considering here, condition (173) becomes

$$f_{c_t c_t}[t, \hat{Q}^{(i)}(t), \hat{c}_t(\mathbf{x}_w, t)] = \sigma^2[\hat{Q}^{(i)}(t) + Q_{LO}] > 0 \tag{216}$$

for all $t \in [t_{i-1}, t_i]$, and for i = 1, 2, 3, and 4. For the constants chosen in this example, the constraint in (216) is met for any choice of i = 1, 2, ... n-1. Since the inequality in (216) holds for every interval, the only test which remains is to verify that the inequality in (212) holds for i = 1, 2, 3, and 4. For example, when i = 1

$$m_{11}^{(1)} = -\frac{1}{2}\left[\hat{f}_{c_t}\hat{c}_{tt}\right]_{x=x_w}\Big|_{t_1+0}^{t_1-0} = -\frac{\sigma^2}{2}\hat{c}_t\hat{c}_{tt}\left[\hat{Q}(t) + Q_{LO}\right]\Big|_{x=x_w}\Big|_{t_1+0}^{t_1-0}, \tag{217}$$

which becomes

$$m_{11}^{(1)} = -\frac{\sigma^2}{2}\left\{\hat{c}_t^-\hat{c}_{tt}^-\left[Q_{ON} + Q_{LO}\right] - Q_{LO}\hat{c}_t^+\hat{c}_{tt}^+\right\}\Big|_{x=x_w}. \tag{218}$$

For the choice of $\hat{c}_t^+ = \kappa_1 \hat{c}_t^-$ and $\hat{c}_{tt}^+ = \kappa_2 \hat{c}_{tt}^-$, where $\kappa_1 = -4.5$ and $\kappa_2 = -2$, (218) reduces to

$$m_{11}^{(1)} = -\frac{\sigma^2}{2} \hat{c}_t^- \hat{c}_{tt}^- \left[Q_{ON} - 8 \cdot Q_{LO}\right]\Big|_{x=x_w}, \tag{219}$$

which is always positive, since $\hat{c}_t^-$ and $\hat{c}_{tt}^-$ are always opposite in sign (Figure 15) and Q_{ON} is greater than $8 \cdot Q_{LO}$. Thus, the $m_{11}^{(i)}$ term is positive for each i = 1, 2, ... n-1, so the matrix $\mathbf{M}^{(i)}$ is nonnegative for any i = 1, 2, 3, and 4.

Returning to Theorem 9, since P(t) is positive for all $t \in (t_{i-1}, t_i) \cup (t_i, t_{i+1})$, and $\mathbf{M}^{(i)}$ is a nonnegative definite matrix, then the functional A in (162) is always positive. Thus, A is a positive definite functional for all h(t) such that $h(t_{i-1}) = h(t_{i+1}) = 0$, and according to the theorem, the interval $[t_{i-1}, t_{i+1}]$ contains no conjugate times to t_{i-1} for every i. With this statement, we have satisfied all the conditions stated in Theorem 10, and as such the pumping schedule (t_1, t_2, t_3, t_4, ...) represents an optimal pumping solution which minimizes the functional defined by (210) and (211), constrained by the appropriate conditions of (25) - (27). □

7.3 *Summary*

This chapter identified general classes of functionals that a remediation site manager might wish to optimize through the use of a pulsed pumping schedule. Several classes were found to either have no optimal pulsed pumping solution, or they could not possibly produce any interesting management objectives. Various other classes were identified as potential candidates for optimization through pulsed scheduling. Necessary optimality conditions which produce a candidate pulsed pumping schedule were

presented for these classes, and several examples served to illustrate the usefulness of the method presented in this document.

The first example depicts a common management goal that a number of researchers have sought to optimize through the use of pulsed pumping. The example clearly demonstrates that an optimal pulsed pumping schedule for the functional in (194) does not exist, and as such, a decision must be made to either pump continually or to not pump at all. Further, this example provides a rigorous proof that pulsed pumping will not maximize remediation goals which reflect an efficiency criteria of contaminant mass removed per volume of water extracted. This conclusion motivated an investigation of the objective functional, which led to new insight into the optimization problem, illustrated in Example 2.

Example 2 demonstrates how the formulation of a realistic objective functional is a key component of the optimization of pump-and-treat operations. The functional in this example suggests that the efforts of previous researchers sought to realize unattainable goals. By adjusting the management criteria to reflect a realistic cleanup goal, a functional was developed and the variational theory was applied, resulting in an optimal pulsed pumping schedule. The schedule was further tested, and we concluded that the candidate schedule was met the objective criteria of the example.

The final example presented yet another twist on the development of realistic objectives. Again, a candidate pulsed pumping schedule was derived and tested and further illustrated the usefulness and flexibility of the variational approach.

The examples presented in this chapter were chosen primarily to illustrate how to use the optimization technique presented in this research. However, through an investigation of the management objective functional, we have depicted the importance of developing attainable management objectives. At the same time, we have demonstrated the utility of this technique and its potential as a cost saving tool for use at pump-and-treat remediation sites.

VIII. Conclusions and Recommendations

8.1 Overview

The remediation and containment of contaminated groundwater remains a persistent ecological problem, and will continue to be an environmental issue in the foreseeable future. Current pump-and-treat methods appear to be most effective as a containment tool, though complete restoration of a contaminated aquifer by use of this technique does not appear feasible. In fact, pump-and-treat water extraction has failed to fully remediate any contaminated aquifer to health-based standards. However, with the prospect of operating a large number of these cleanup facilities for the next 50 to 100 years, research into minimizing operating costs has received a great deal of attention. The research presented in this dissertation employs calculus of variations techniques, seeking to minimize a generic management objective functional by finding the optimal switching times for a schedule of pulsed pumping operations.

The literature reviewed supports pulsed pumping as a method to minimize costs at pump-and-treat cleanup sites by reducing the volume of contaminated water to be treated, especially at sites where rate-limited sorption is evident. However, most of the investigations of pulsed pumping were conducted using arbitrary or trial-and-error methods to determine a pulsed schedule, and only Hartman (1994) sought to use an analytical optimization technique to find an optimal pulsed pumping solution. Hartman's work was a very restricted component of a much more complex problem, and the present

research used a similar technique, but on a more general setting which led to a more thorough analysis of the problem.

8.2 *Summary of Findings*

The goal of this research was to develop necessary and sufficient conditions for an optimal pulsed pumping schedule in order to minimize a generic management objective functional, constrained by the physical properties of the given model. The Lagrangian, developed in Chapter III, combined the objective functional with the constraints represented by the equations for advective-dispersive contaminant transport, coupled with the first-order rate-limited sorption equation. Specifically, a calculus of variations approach was applied to the Lagrangian, resulting in conditions which must be met by any pulsed pumping schedule which minimizes the objective.

This variational method resulted in a set of necessary and sufficient conditions that, when combined with concentration information, provided a rigorous means of finding optimal pulsed pumping solutions. The approach incorporated a very general functional that allowed maximum flexibility in specifying management objectives. Examples 2 and 3 illustrated how a properly chosen objective could be translated into a realistic functional. This functional, in turn, could be transformed into manageable conditions using the theorems developed in earlier chapters. This coupling of management input with the mathematical rigor developed in this document is a major asset to the work. The following is a list of specific contributions produced through the course of this research:

1. Chapter IV applied the theory of the first variation of the Lagrangian, and developed a necessary conditions theorem which served to establish a candidate pulsed pumping schedule. This candidate schedule depends on the concentration and its time derivatives at the well, but not on the Lagrange multiplier, which was introduced in equation (37). Theorem 6 must be satisfied by any pulsed pumping schedule that minimizes the functional and constraints presented in Chapter III.
2. Chapter V applied the theory of the second variation of the Lagrangian and developed a necessary conditions theorem which assured a minimal solution for the optimization problem, provided the necessary conditions of Chapter IV are met. Additionally, these necessary conditions served to motivate the theorems that provided sufficiency for a minimum, presented in Chapter VI.
3. Chapter VI developed the proofs of two theorems which provide an exhaustive list of necessary and sufficient conditions, which if met, guarantee a minimal solution to the optimization problem presented in Chapter III. These conditions can be used as tests for any particular objective functional to determine the validity of employing a pulsed schedule of operation.
4. Chapter VII served to demonstrate how the tests, developed through the analysis of the previous three chapters, can be employed in conjunction with discrete concentration information at the extraction well (provided by any numerical model which incorporates first-order rate-limited sorption). Additionally, the examples highlighted the simple use of these conditions that at first glance appear difficult to manage. While the examples in Chapter VII were designed to demonstrate the utility

of the method, two significant results emerged from the investigation. Example 1 puts to rest an argument that has occupied investigators for some time. Several authors have repeatedly sought to demonstrate either the utility or futility of pulsed pumping in a rate-limited sorption environment. Their investigations have amounted to searches of the solution space of pumping schedules, some of which have numbered in the tens of thousands (Harvey, et al., 1994). Example 1 provided rigorous proof for the first time that pulsed pumping will not maximize the benefit when the criteria for efficiency is contaminant mass removed per volume of water pumped. Example 2 also provided new insight into the problem of optimizing pump-and-treat remediation. In this example, the formulation of the objective functional emerged as a key factor in the optimization problem. The functional in this example suggested that previous researchers may have been looking at the wrong remediation goal. Restoration to pristine aquifer conditions is not realistically achievable. The generality of the results developed in this research allowed for exploration of different management objectives, and Examples 2 and 3 suggested new approaches to establishing cleanup objectives.

8.3 Recommendations

This research has provided the mathematical analysis for establishing pulsed pumping schedules for use at existing pump-and-treat facilities, where the contaminant transport is effected by rate-limited sorption. Some simplifying assumptions were made to facilitate the analysis and illustrate the use of tests presented in Chapter VI.

Recommendations for further research are directed toward eliminating these assumptions. Specifically, continuation of this research should focus on the following areas:

1. A more general approach to modeling rate-limited sorption should be pursued. In this research, a first-order model was assumed early on, since the majority of production codes in use assume a first-order model for desorption of contaminant from less mobile regions. Further generalizing the sorption model (i.e., second-order models incorporating diffusion, mixed models, etc.) would make the analysis more usable for attaining management objectives at a greater variety of remediation sites. As stated in Chapter VII, the examples were used primarily to demonstrate the potential of the optimization technique presented in this document. However, two significant results documented above were a side benefit of these examples. Example 2 clearly demonstrated the impact of choosing a functional with realistic physical significance. Further studies should pursue the development of appropriate functionals for optimizing pump-and-treat remediation. This effort should be a collaboration between hydrologists, environmental engineers, and applied mathematicians employing the theory developed in this document to quickly demonstrate the utility of each functional.

2. In Examples 2 and 3, a numerical approximation for the first and second time derivatives of the concentration was used to illustrate the method. Also, a simplifying assumption was made about the relationship between the derivatives before and after the status of the pump switches. In practice, we would need a better approximation for these terms and a better way to predict their behavior immediately after the pump

changes status. Finding an analytical solution for the first time derivative of the concentration at the well would be a logical next step. Specifically, one could prove that there exists some function $\psi(t,c)$ such that $c_t^{(i+1)}(t,\mathbf{x}_w) = \psi(t, c^{(i)}(t,\mathbf{x}_w))$, and then this approximation would become exact.

3. Implementing this procedure using data from an extraction well at an actual treatment site would also be appropriate.
4. Move the monitoring location away from the extraction point, and possibly several different monitoring locations.
5. Allow for several extraction wells, where one pumping schedule might depend on the other pumps.
6. Add objective functionals to J[Q,c] that relate to contaminant containment, to determine how one should pump so that contaminant is contained, and at the same time, remediation is optimal.

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Vita

Capt Lawrence J. Schmitt was born on 29 December 1958 in Hamilton! Ohio. He graduated from Hamilton Garfield High School in 1977 and enlisted in the United States Air Force in 1978. After spending six years working at Wright-Patterson AFB as a plumbing specialist, he was accepted into the Airmen's Education and Commissioning Program and attended Wright State University where he graduated Summa Cum Laude with a Bachelor of Science degree in Electrical Engineering in March 1987. He received his commission on 26 June 1987 when he completed Officer Training School as a Distinguished Graduate.

Capt Schmitt's first assignment as an officer was at Patrick AFB where he worked as a Program Support Manager for the Air Force Titan launch system, and he also served as Range Control Officer for 17 Department of Defense and NASA orbital and ballistic launch operations. While at Patrick, he was selected for a Faculty Preparation assignment for instructor duty at the United States Air Force Academy, which he completed by earning the degree of Master of Science in Applied Mathematics from the Florida Institute of Technology in March 1992. From May 1992 to August 1994 he was assigned to the Department of Mathematical Sciences at the Academy, and he was chosen as the 1994 winner of the Tony M. Johnson award, the department's annual award for mathematics teaching excellence. In September of 1994 he entered AFIT's School of Engineering as a Ph.D. student in the Department of Mathematics and Statistics.

Captain Schmitt is married to the former Marianne Rief of Dayton, Ohio. They have four children: Carolyn, age 11; Katie, age 9; Laura, age 7; and Timmy, age 5.

Following his graduation from AFIT, he will be assigned to the Wright Laboratory at Wright-Patterson AFB Ohio.

Permanent Address: 6621 Loblolly Drive
Huber Heights, Ohio 45424

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A variational optimization technique is developed to acquire an optimal schedule of pulsed pumping operations for use at existing pump-and-treat aquifer remediation sites. The optimization problem is stated as a minimization of a generic management objective functional, constrained by the contaminant transport equations in two-dimensional or three-dimensional flow models which account for rate-limited sorption. The two-dimensional case is fully developed and a first-order rate equation is used to describe the transport of sorbing contaminant. The first variation provides necessary optimality conditions that must be met by any optimal solution, in turn leading to a pulsed pumping schedule of operation. The second variation provides necessary and sufficient optimality conditions that characterize the solution as minimal, maximal, or neither. General classes of functionals are examined to determine the types of objectives which can be achieved. Specific examples are presented to demonstrate how to use the method in conjunction with a numeric flow simulation, such as SUTRA.

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